



## **A risk assessment tool for contaminated sites in low-permeability fractured media**

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**Chambon, Julie Claire Claudia; Bjerg, Poul Løgstrup; Binning, Philip John**

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# A risk assessment tool for contaminated sites in low-permeability fractured media

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A risk assessment tool for contaminated sites in low-permeability fractured media

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# Preface

This report presents the development of a risk assessment module for contaminated fractured media for implementation in JAGG2.0. The tool is based on analytical solutions and is implemented in Microsoft Excel 2007. This report illustrates the use of the developed tool with several case studies. The performance of the risk assessment tool compared to other approaches is also discussed.

The project is conducted by Julie Chambon, Philip J. Binning and Poul L. Bjerg from DTU Environment and financed by Miljøstyrelsens Teknologiprogram for jord- og grundvandsforurening.

Review of the project work and the report has been done by a steering group. The chairman of the group was Ole Kiilerich (Miljøstyrelsen), and group members were Arne Rokkjær (Region H) and Thomas Hauerberg Larsen (Dansk Miljørådgivning).

The authors would like to thank Peter R. Jørgensen for kindly providing data from Skælskør and for discussions and helpful suggestions during the work.



# Sammenfatning og konklusioner

I Danmark findes mange forurenede grunde i områder med lav-permeable opsprækkede aflejringer (fx moræneler). Forureninger kan transporteres hurtigt til den underliggende akvifer gennem preferentielle strømningsveje dannet af sprækker, men kan også diffundere in i selve den porøse matrice. Opsprækkede aflejringer er vigtige at tage højde for ved vurdering af risiko for grundvandsforurening på forurenede grunde på grund af den hurtige nedadrettede transport, og den store kapacitet for lagring af forurening i den porøse matrix.

En sprækkemodel (SprækkeJAGG) til forudsigelse af vertikal transport fra en forureningskilde til en underliggende akvifer er tidligere blevet udviklet til det danske risikovurderingsværktøj JAGG. SprækkeJAGG er i dette studium yderligere blevet udviklet med fokus på vand balancen for et opsprækket medium, udvikling af transiente analytiske løsninger for forskellige geometrier og historie af forureningskilden, koblingen til den underliggende akvifer og den eksisterende JAGG model.

Det udviklede værktøj (som er et modul i JAGG2.0 og i denne rapport benævnt JAGG2.0) er blevet testet på et bredt udsnit af datasæt fra videnskabelige undersøgelser, og brugen af risikovurderingsværktøjet er illustreret med adskillige eksempler med relevante stoffer for forurenede grunde i Danmark. De mange eksempler er brugt til at illustrere risikovurderingsværktøjets anvendelse men også til at sammenligne det med en simplere model, den såkaldte ækvivalente porøse medium model (Equivalent Porous Media, EPM). EPM modellen tager ikke explicit højde for tilstedeværelsen af sprækker. På baggrund af sammenligningen mellem de to model tilgange er der givet anbefalinger vedrørende brugen af en sprækkemodel ved risikovurdering af forurende grunde.

Risikovurderingsværktøjet er baseret på to konceptuelle modeller for forureningskildens geometri. Model 1 repræsenterer en forureningskilde liggende over et opsprækket medium med en konstant koncentration i enten en uendelig tid (1a) eller i et kendt tidsrum fx ved fjernelse af en tank (1b). Model 2



repræsenterer forureningskilden med en homogen koncentrationsfordeling i selve den porøse matrix i det porøse medium. Simple analytiske løsninger for transiente forhold og ved steady state er udviklet baseret på Tang et al. (1981) og Sudicky and Frind (1982). Løsningerne er implementeret i et brugervenligt Excel regneark. Adskillige forenklinger har været nødvendige for at udvikle de analytiske løsninger. Først og fremmest er et netværk af vertikale sprækker forenklet til én vertikal sprække omgivet af en semi-uendelig matrice. Dette betyder, at risikoen undervurderes for model 1 ved små sprækkeafstande, mens de to systemer opfører sig identisk ved sprækkeafstande på mere end 1 m. Risikoen er overvurderet for model 2, da forureningskilden i den porøse medium bliver uendelig. Vandstrømningen i det opsprækkede medium er antaget til at være konstant. Det kan betyde, at risikoen undervurderes ved voldsomme regnhændelser med hurtig nedadrettet strømning i sprækken til akviferen. Det er yderligere antaget, at den porøse matrice er impermeabel (vandstrømning sker kun i sprækken). Den simplificering af vandstrømningen betyder, at risikoen er overvurderet for model 1 på grund af hurtigere strømning gennem sprække, og undervurderet for model 2 på grund af forøget fortynding i sprækken.

JAGG2.0 er afprøvet på flere kolonne og felteksperimenter med konservative og reaktive stoffer fx bromid, klorid, MCPP og vira. Modellen simulerer de eksperimentelle data godt, og den simple EPM model kan ikke tilpasses til de målte data med realistiske parametre. Alle disse eksperimenter er udført under velkontrollerede forhold og forsøgene er af kort varighed. Fokus i forsøgene har været at demonstrere det hurtige gennembrud gennem et opsprækket medie, hvilket er lykkedes at beskrive med den udviklede model. Udsivning over lang tid, som er forventet på grund af den oplagrede forurening i matricen, er ikke dokumenteret med de eksperimentelle data med undtagelse af eksperimenter ved Flakkebjerg, hvor fortolkning med en simpel analytisk model er vanskelig.

Anvendelsen af JAGG2.0 til risikovurdering er illustreret med en række eksempler fra forurenede grunde i Danmark. Udsivningen fra diffuse forureningskilder (Hvidovre) og punktkilder (Skælskør) er undersøgt med modellen. Tilstedeværelsen af BAM i grundvandet og i vandforsyningsboringer omkring Hvidovre vandværk og ved en punktkilde i Skælskør er velbeskrevet med modellen. JAGG2.0 rammer den rette størrelsesorden af de

målte koncentrationer. Det er muligt at beskrive varigheden af BAM forureningen i Hvidovre, som er forventet at fortsætte til 2050 (med en koncentration  $>0.1 \mu\text{g/L}$ ). Det er demonstreret, at EPM modellen også kan simulere de observerede koncentrationer fra 1995-2008 med realistiske parameterverdier. Det er derfor ikke muligt ved sammenligning med de tilgængelige data at træffe et valg mellem sprækkemodellen eller EPM modellen.

JAGG2.0 er også anvendt til at vurdere risikoen fra et DNAPL spild med chlorerede opløsningsmidler ved en opsprækket morænelerslokalitet på Sortebrovej, Fyn. Koncentrationen i det forurenede område og i den øvre akvifer er velbeskrevet med modellen. Koncentrationen i den regionale akvifer og på vandværket er også vurderet, og det er vist, at koncentrationen vil overstige grundvandskvalitetskriteriet i de kommende år. Resultaterne fra modellen svarer rimeligt til en mere kompleks numerisk model for lokaliteten.

Afslutningsvis er JAGG2.0 anvendt på et eksempel fra en benzinstation (MTBE og benzen). JAGG2.0 resultater blev sammenlignet med resultater fra JAGG1.5. For MTBE som regnes konservativt overestimerer JAGG1.5 risikoen sammenlignet med JAGG2.0, som tager højde for transient vertikal transport. For benzen, som antages at blive nedbrudt under den vertikale transport til akviferen, overestimerer JAGG1.5 risikoen, da nedbrydning ikke er inkluderet i JAGG1.5.

Eksemplerne viser anvendelsen af JAGG2.0 i forskellige situationer for forskellige stoffer. Det har ikke været muligt at vise, at JAGG2.0 modellen er bedre end den simple EPM model ved anvendelse af feltdata. Det skyldes manglen på data for de lange tidshorisonter på de forurenede grunde. I en risikovurdering, er en af de vigtigste overvejelser at sikre konservative resultater, da der er betydelig usikkerhed på parametre og processer. Sammenligning mellem EPM og JAGG2.0 viser, at JAGG2.0 er mere konservativ for nedbrydelige stoffer, da reduktionen i koncentration ved nedbrydning er overvurderet i EPM modellen. Det er også vist, at EPM modellen for ikke-nedbrydelige stoffer forudsiger højere koncentrationer end JAGG2.0.

Det er anbefalet ved risikovurdering at anvende model 1a, når en forureningskilde kan identificeres, og forureningskoncentrationen kan måles. I det tilfælde, hvor forureningskilden ikke kan findes,

anbefales det at anvende model 2, hvor de målte koncentrationer i det opsprækkede medium anvendes.

# Summary and conclusions

In Denmark many contaminated sites occur in areas with low-permeability fractured media (such as clay-rich glacial deposits) at the land surface, where contaminants can migrate rapidly to the underlying aquifer through the preferential pathways formed by the fractures and are stored via diffusion into the adjacent porous matrix. Fractured media is important to consider when assessing risk to the groundwater at contaminated sites, because of the fast downward pathway along the fractures and the high-contaminant-storage capacity formed by the porous matrix. A fracture model (SprækkeJAGG) which aims to predict the vertical transport from a source zone to an underlying aquifer has previously been developed for the Danish risk assessment tool JAGG. This model has been further developed in this study with particular focus on the water balance in fractured media, the development of transient analytical solutions for different source geometries and history, the coupling to the underlying aquifer and to the existing JAGG.

The tool developed in this study (which is a module of JAGG2.0 and is referred in this report as JAGG2.0) has been tested on a wide range of scientific datasets, and the use of the risk assessment tool is illustrated by several case studies involving a range of contaminants commonly found at Danish contaminated sites. The case studies are used to illustrate the risk assessment tool and to compare its performance with a simpler model approach, the Equivalent Porous Media (EPM), which does not explicitly account for the presence of fractures. The comparison between the two approaches forms a basis for recommendations on the use of a modeling tool for fractured media in risk assessment of contaminated sites.

The risk assessment tool is developed based on two conceptual models for the source geometry. Model 1 represents the source overlying the fractured media, with a constant concentration, for either infinite time (1a), or for a known duration (1b) such as when a source from a leaking tank is removed. Model 2

represents the source stored in the porous matrix of the fractured media, with a uniform concentration. Simple transient and steady state analytical solutions are developed based on the work of Tang et al. (1981) and Sudicky and Frind (1982). The solutions are implemented in a “user-friendly” Excel sheet. Several simplifications have been necessary in order to obtain the analytical solutions. First, the network of parallel vertical fractures is simplified to a single fracture surrounded by a semi-infinite matrix. This results in an underestimation of the risk for model 1 for small fracture spacing, but the two networks become equivalent for fracture spacing greater than 1 m. The risk is overestimated for model 2, as contaminant source located in the fractured media becomes infinite. The flow in the fractured media is assumed to be constant. This can lead to an underestimation of the risk in case of extreme event with fast downward flow along the fractures to the aquifer. Furthermore the porous matrix is assumed to be impermeable (water flows along the fractures only). With this simplified description of the water flow, the risk is overestimated for model 1 due to the faster flow through the fracture, and underestimated for model 2 due to a faster dilution in the fracture.

JAGG2.0 is applied to several column and field experiments involving conservative and reactive compounds, such as bromide, chloride, MCPP and viruses. The model simulates the experimental data well, and it is shown that the simpler EPM approach cannot fit the measured data with realistic parameters. However these experiments have been conducted under well-controlled conditions and are of short duration. The focus of the experiments was to demonstrate the fast breakthrough through the fracture network, which is well captured by the developed model. But long term leaching that is expected due to high storage capacity in the porous matrix is not documented by experimental data, except for an experiment at Flakkebjerg, where the interpretation with a simple analytical model is difficult.

The use of JAGG2.0 for risk assessment purposes is illustrated with several case studies involving Danish contaminated sites. The leaching to the aquifer from diffuse and point sources of pesticides is studied with the model. The presence of pesticides (BAM) in the groundwater and waterworks around Hvidovre, as well as in the aquifer below the point source in Skælsør is well predicted by the model results. JAGG2.0 captures the

order of magnitude of the measured concentrations. It is possible to estimate the duration of the contamination; the presence of BAM in Hvidovre waterworks is expected until 2050 (with a concentration  $>0.1 \mu\text{g/L}$ ). It is also shown that the EPM model can simulate the observed concentrations for the period 1995-2008 using realistic parameter values. For this example it is therefore not possible to conclude which model is better able to simulate the data.

JAGG2.0 is also used to assess the risk posed by a DNAPL spill of chlorinated solvents over a fractured clay till at Sortebrovej, Fyn. The concentrations in the source zone and the upper aquifer are well simulated by the model. Furthermore the concentrations in the regional aquifer and the waterworks are estimated, and it is shown that the concentrations in the waterworks are expected to exceed drinking limits for many years in future. The results from the risk assessment tool JAGG2.0 (fracture module) also compare reasonably well with a complex numerical model developed for the site.

Finally JAGG2.0 is applied to the case of MTBE and benzene contamination from a gas station. JAGG2.0 results are compared with the results from JAGG1.5. For the conservative compound (MTBE), JAGG1.5 overestimates the risk compared with JAGG2.0, which takes into account the transient vertical transport. For the case of benzene, which is assumed to degrade during the vertical transport to the aquifer, JAGG1.5 overestimates the risk (as degradation is not included).

The case studies show the applicability of JAGG2.0 for several situations and compounds. However it was not possible to fully verify the model compared to the simpler EPM approach using field observations. This is due to lack of data for long timeframes at contaminated sites (due to the low-permeability matrix). In a risk assessment context, one of the most important considerations is to ensure that conservative results are obtained, given the high uncertainty on the parameters and processes. The comparison between EPM and JAGG2.0 shows that JAGG2.0 is more conservative for degradable compounds, because the attenuation is overestimated for EPM model. However it is also shown that for non-degradable compounds, EPM model predicts higher concentrations than JAGG2.0.

To perform risk assessment, it is recommended that model 1a is used when a source can be identified and concentrations in

the source can be measured. In the case where the source cannot be found, model 2 should be applied, using measured concentration in the fractured media.

# 1 Risk assessment for contamination located in fractured media

## 1.1 Overview

Low-permeability fractured media is a common geology in Denmark, where glacial deposits of clay-rich till covers most of the land surface (Jørgensen et al. 2002). Many contaminated sites occur in such areas, where the high heterogeneity of the geological formation results in complex transport processes: contaminants can penetrate rapidly to the underlying aquifer through the preferential flow pathways formed by the fractures and can also diffuse to the adjacent porous matrix. Hence accounting for fractured media is an important issue when assessing risk to the groundwater at contaminated sites, because of the fast downward pathway along the fractures and the high-contaminant-storage capacity of the porous matrix. Several examples of such sites can be found in Denmark, involving contaminants such as chlorinated solvents, creosotes, BTEX and pesticides.

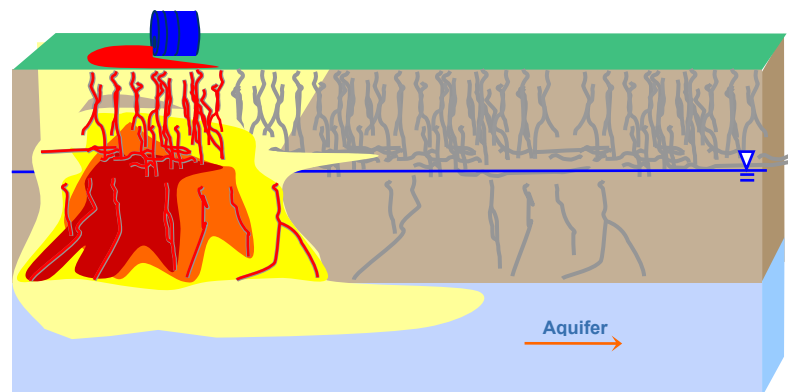


Figure 1 – Contaminant transport in low-permeability fractured media: fast downward transport to the aquifer along the fractures and diffusion into the adjacent porous matrix

## 1.2 Risk assessment

### 1.2.1 Existing tools

In most screening tools for risk assessment (such as JAGG1.5, RISC Workbench 4.0), transport through fractured media is very



simplified. In general the fractured media is considered as an equivalent porous media (EPM) with equivalent hydraulic conductivity and porosity. Although such simplifications are valid in some cases, particularly for small fracture spacing (van der Kamp 1992, McKay et al. 1997), transport processes in low-permeability fractured media are much more complicated. The migration of contaminants is controlled by advection in the fracture, exchange between the fracture and the matrix and molecular diffusion in the low-permeability matrix. In addition degradation processes for organic contaminants add to the complexity. EPM models are expected to misjudge the risk posed to groundwater by overestimating the breakthrough times, the attenuation by degradation and underestimating the leaching times.

Recently a risk assessment tool for low-permeability fractured media has been developed (Excelsheet SprækkeJAGG, Videncenter for Jordforurening 2008). The tool calculates the steady-state contaminant leaching from a fractured clayey till under constant input source condition. However several types of contaminated sites are not well described by the conceptual model of SprækkeJAGG, and further development of a risk assessment tool for low-permeability fractured media is required.

#### **1.2.2 Purpose of the risk assessment tool**

A risk assessment tool is intended to be used to characterize the risk posed by contamination to the groundwater resource at a particular contaminated site. This means that the leaching rate from the contaminated source area into the groundwater and the contaminant concentrations are calculated. The concentration can be compared with quality standards in order to evaluate the risk. However it is also interesting to evaluate the leaching rate as a function of time: is it expected to increase/decrease, last for decades, ...? The risk assessment tool therefore calculates the evolution of contaminant leaching with time.

For practical purposes the risk assessment tools should be user-friendly and the data requirement should be as limited as possible, therefore the model preferably should be based on analytical solutions and implementable in Excel.

#### **1.3 Analytical solutions**

Many analytical solutions are available for simulating contaminant transport in a single or parallel fractures system, accounting for

advection and dispersion along the fracture, molecular diffusion and adsorption within the matrix, as well as first order radioactive decay in both the fracture and matrix. Tang et al. (1981) and Sudicky and Frind (1982) developed the transient analytical solution for a single compound in a single and parallel fractures system respectively, for the case of a constant input source. The single fracture solution was further developed to include reactive transport of a two-member decay chain by Sudicky and Frind (1984) and a N-member decay chain by Sun and Busheck (2003) for pulse injection and constant input source. Chen and Li (1997) developed an analytical solution for a system of parallel fractures with a constant inlet flux. Analytical solutions for other input sources (single pulse and sinusoidal input source) were developed by Shih et al. (2002), but for the case with negligible matrix diffusion. All of these solutions are intended for radioactive compounds, subject to uniform decay in both the dissolved and the sorbed phases. Very limited work has been done for chemical and biological reactions in fractured media (Schmelling and Ross 1996). However most of the relevant compounds at contaminated sites (hydrocarbons, chlorinated solvents...) can undergo biological degradation, which occurs primary in the aqueous phase. Furthermore specific solutions with relevant initial concentration distributions and certain boundary conditions are lacking in the literature for risk assessment at contaminated sites.

#### 1.4 Objectives

The project aims to develop a risk assessment tool for contaminated sites in low-permeability fractured media. This tool, which is based on analytical solutions, should provide both steady-state and transient outputs. The developed tool will be implemented in a “user-friendly” interface in Excel. Furthermore the tool should be coupled to the new version of the global Danish risk assessment tool JAGG2.0, and provide prediction of the contaminant concentration in the underlying aquifer.

In order to validate the model, the tool is applied to a number of scientific examples. The tool is also applied to several case studies to illustrate its use as a risk assessment tool. The case studies are chosen to cover a range of contaminants commonly found in Denmark.

The validity and advantages of a specific risk assessment tool for fractured media are discussed, particularly when compared to the simpler equivalent porous media (EPM) model. The

comparison is based on the case studies, and a discussion of model predictive uncertainty and its impact on risk evaluation, i.e. when should conservative model assumptions be applied.

## 2 Conceptual models for fractured clay aquitards

A set of conceptual models is developed in order to represent the different situations for contamination sources typically found in Denmark in low-permeability fractured media. The conceptual models are based on existing contaminated sites in Denmark.

### 2.1 Conceptual models of fractured clay till

The physical system considered in this study is illustrated in Figure 1a with a low-permeability fractured media overlying an aquifer. The developed risk assessment tool focuses on the fractured media in the saturated zone, and so the transport of the gas phase is not included. In some conditions the model can also be applied in the unsaturated zone, for instance when clays are above the water table but remain saturated due to capillary forces. The complex fracture network embedded in the low-permeability settings is simplified in Figure 1b, where only fully penetrating vertical fractures are taken into account and a homogeneous fracture spacing is assumed. These simplifications of the natural network are motivated by the scope of this study, which focuses on risk assessment posed to the underlying aquifer by downward transport through the fractured media, so the horizontal features are of less importance. The geometry is further simplified and only considers a single fracture surrounded by a semi-infinite matrix. In case of large fracture spacing, this simplification is reasonable. The validity and limitations of the single fracture assumption is discussed in Section 9.3. All conceptual models considered are based on this general physical description and only vary with differing boundary and initial conditions.

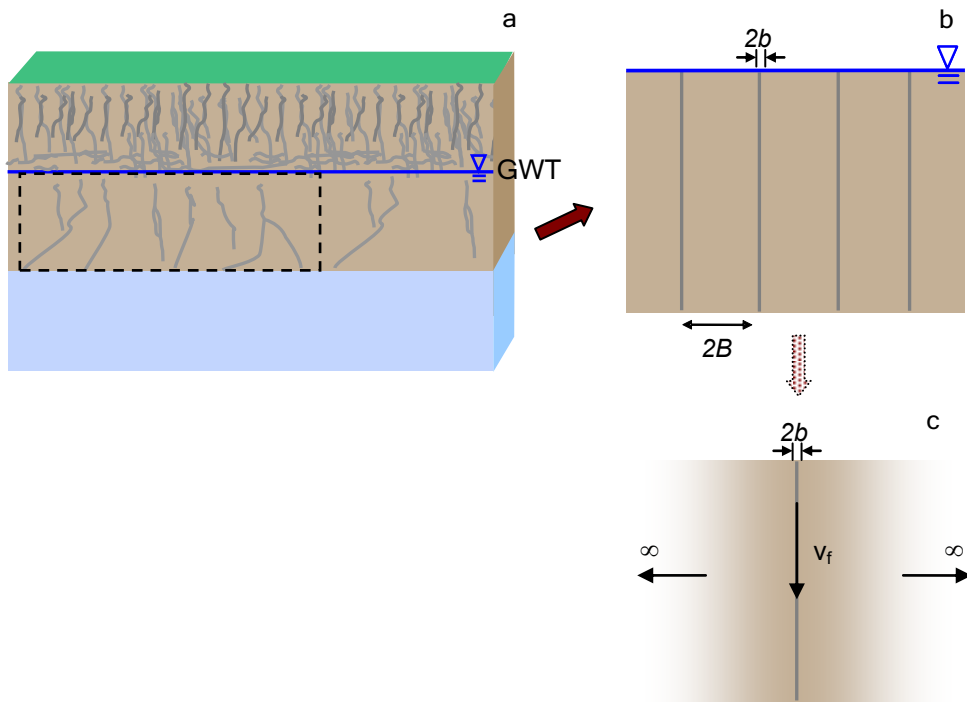


Figure 2 – a) Physical system considered in this study: a low-permeability fractured media overlies an aquifer. The area of interest located in the saturated zone is shown with the dashed box. b) Simplification of the fractured media for modeling: the fractures are assumed to be fully penetrating and equally spaced. c) Further simplification with the case of a single fracture embedded in a semi-infinite porous matrix

Two types of source are modeled in this report. In the first the contaminant overlies a fractured clay aquitard, while in the second, the source has been removed, but contaminant is trapped in the clay below the former source continues to leach for many years afterwards. There are described in the sections below.

## 2.2 Model 1: Source overlying a low-permeability fractured media

Contaminated sites where contaminant source overlies a low permeability fractured media is common in Denmark, for example in case of pesticides spreading on agricultural soil, oil tank leaking to the underlying fractured media, DNAPL release at the land surface, etc... The conceptual model is illustrated in Figure 3.

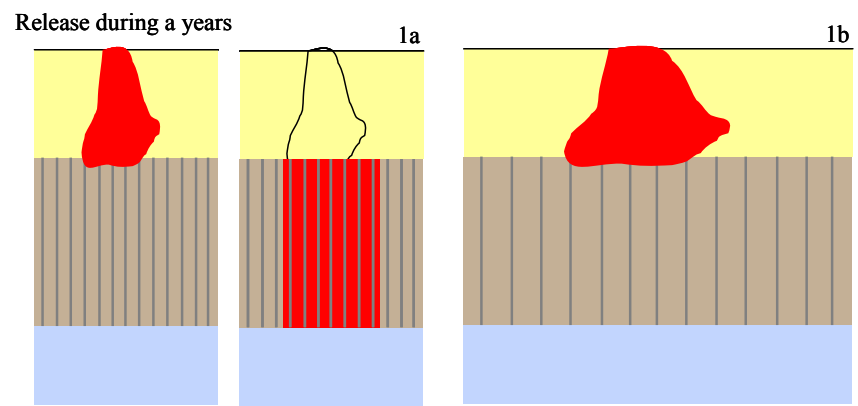


Figure 3 – Source overlying a low-permeability fractured media

Two input sources are considered for this model:

- Model 1a: Input source with constant concentration  $C_0$  for a known period of time ( $a$  years) before removal
- Model 1b: Constant input source with concentration  $C_0$

The model 1b is a specific case of 1a, where the contaminant source has not been removed.

### 2.3 Model 2: Contaminated fractured till leaching to the underlying aquifer

In many cases the contamination source (such as tank, pipe, reservoir) has been removed from the sites and the history of contamination (amount, length, concentration, geometry) of the fractured media is unknown. In such cases the measured concentration in the porous matrix and the contaminant mass present in the low-permeability media are the only available data. An illustration of such a case is the site at Kongevej 39, where the fractured clayey till overlying the chalk aquifer is contaminated with chlorinated solvents (Miljøkontrollen 2004a). The contaminant source has been removed and the former industrial site is replaced by a parking lot. The contaminated fractured media acts as a contaminant source for the underlying chalk aquifer with the chlorinated solvents leaching slowly downwards. This case can be modeled with a zero input concentration at the top of the fracture and a homogeneous initial concentration in the porous matrix (see Figure 4).

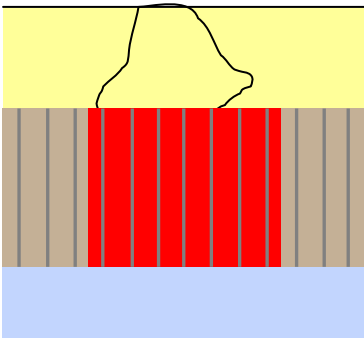


Figure 4 – Contaminated fractured media overlying the aquifer

### 3 Groundwater risk assessment

The fracture module of JAGG2.0 developed in this report is intended to evaluate the concentration of contaminants leaching from a clay aquitard to an underlying aquifer. In this chapter, the general use of the model to assess risk posed to the underlying aquifer is discussed. The coupling of the developed tool to JAGG1.5 is presented in the chapter 4.

#### 3.1 Flux to the underlying aquifer

The contaminant flux resulting from the fractured media is coupled to the groundwater model using following conceptual model is used:

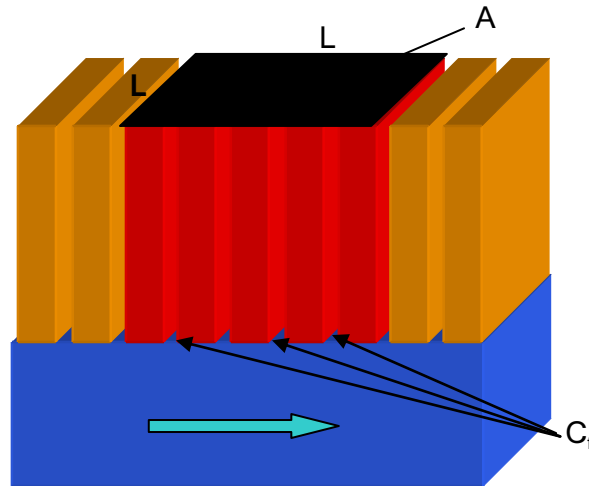


Figure 5 – Conceptual model for fractured media and underlying aquifer

The contaminant source is assumed to have a square shape, with an area  $A = L^2$ . The number of fractures in the source zone is then:

$$nb = \frac{L}{2B} \quad (3.1)$$

It has to be noticed that in contrast to JAGG1.5, the source is assumed to have a quadratic shape (and not rectangular),  $A = L * L$ .

The contaminant discharge from one single fracture is:



$$J_{frac} = C_f \cdot v_f \cdot 2b \cdot L \quad (3.2)$$

Where  $C_f$  is the concentration at the fracture outlet ( $M/L^3$ ),  $v_f$  is the velocity in the fracture ( $L/T$ ) and  $2b$  is the fracture aperture ( $L$ ).

Assuming a complete mixing of the contaminated flux from the different fractures, the total flux from the source is:

$$J_{source} = C_f v_f 2b \cdot A / 2B \quad (3.3)$$

Which can be written using the net infiltration rate through the fractured media ( $I$ ):

$$J_{source} = C_f \cdot A \cdot I \quad (3.4)$$

$C_f$  is the concentration calculated with the model for the depth corresponding to the fractured layer thickness.

### 3.2 Concentration in the aquifer

Based on the above assumption of a mixed homogeneous contaminant flux from the fractured media, the concentration in the underlying aquifer can be estimated based on the dilution factor model (DAF) (Miljøstyrelsen 1998):

$$C_{aq} = \frac{J_{source}}{F_{aq}} = \frac{C_f A I}{A I + K_{aq} i_{aq} d_m L} = \frac{C_f}{DAF} \quad (3.5)$$

where  $DAF = 1 + \frac{K_{aq} i_{aq} d_m}{IL}$

Where  $K_{aq}$  is the hydraulic conductivity of the aquifer ( $L/T$ ),  $i_{aq}$  is the hydraulic gradient in the aquifer and  $d_m$  is the mixing zone depth, which can be calculated according to the guidance in Miljøstyrelsen (1998).

In this study, the filter length of monitoring wells is used for  $d_m$  for comparison with field data.

### 3.3 Concentration in surrounding drinking wells

Assuming that all the contaminated groundwater in the aquifer is pumped by the surrounding drinking wells and that no degradation takes place during transport in the aquifer, the concentration in the wells can be estimated (Trolborg et al. 2008):

$$C_{well} = \frac{J_{source}}{Q_{well}} = \frac{A \cdot I \cdot C_f}{Q_{well}} \quad (3.6)$$

where  $Q_{well}$  is the annual pumping rate of the waterworks.

In this simple model, the travel time from the source zone to the waterworks and the mass losses due to diffusion into low conductivity layers are not taken into account (Trolborg et al. 2008).

### 3.4 Catchment scale risk assessment

The contaminant discharge from the fractured media (cf. Eq.(3.4) ) can be used to perform catchment scale risk assessment and site prioritization. For example the analytical solution can be coupled to CatchRisk model (Trolborg et al. 2008), and a risk assessment for the regional groundwater and the surrounding drinking wells can be performed based on travel time and particle tracking.

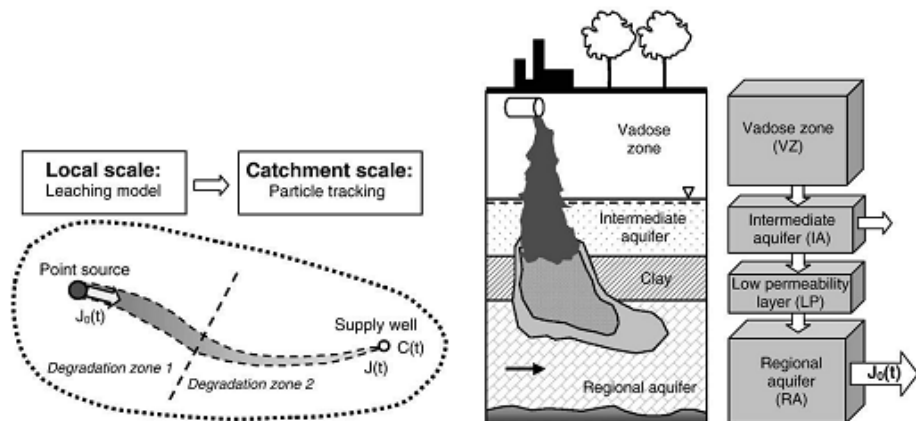


Figure 6 – CatchRisk model (right) and leaching model (left), from (Trolborg et al. 2008). The fractured model can be incorporated in the leaching model instead of the "Vadose Zone" box



## 4 Coupling with groundwater module in JAGG

This chapter describes briefly how the developed module for fractured media is coupled with the groundwater module in JAGG to perform risk assessment in the underlying aquifer.

Based on the assumption of a mixed homogeneous contaminant flux from the fractured media, the fracture model is coupled with the groundwater module in JAGG to estimate the resulting concentration in an underlying aquifer. The source concentration in JAGG (“Kildestyrekoncentration”) is replaced by the concentration at the fracture outlet calculated from the model,  $C_f$ .

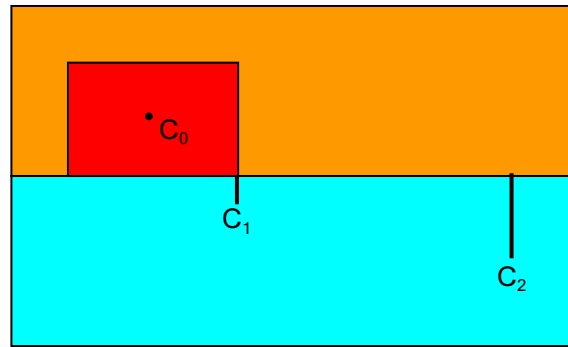


Figure 7 – Conceptual model in JAGG

The concentration in the aquifer at the corner of the source ( $C_1$ ) is calculated in Trin IA in the groundwater module with Eq.(4.1), where the source concentration  $C_0$  is replaced by the concentration at the fracture outlet  $C_f$ .

$$C_1 = \frac{A \cdot I \cdot C_f + L \cdot 0.25 \cdot K_{aq} \cdot i_{aq} \cdot C_g}{A \cdot I + L \cdot 0.25 \cdot K_{aq} \cdot i_{aq}} \quad (4.1)$$

Where  $K_{aq}$  is the hydraulic conductivity in the aquifer,  $i_{aq}$  is the horizontal hydraulic gradient,  $C_g$  is the background concentration,  $A$  is the contaminated area,  $L$  is the length of the contaminated area along the groundwater flow direction and  $I$  is the net infiltration. Note that the source is assumed to be square in this model, with  $A = L \cdot L$ .

The concentration in the aquifer at a distance of one-year from the source is calculated in Trian IIA in the groundwater module with Eq.(4.2), where the source concentration  $C_o$  is replaced by the concentration at the fracture outlet  $C_f$

$$C_2 = \frac{A \cdot I \cdot C_f + L \cdot d_m \cdot K_{aq} \cdot i_{aq} \cdot C_g}{A \cdot I + L \cdot d_m \cdot K_{aq} \cdot i_{aq}} \quad (4.2)$$

Where  $d_m$  is the mixing zone depth calculated by the groundwater module in JAGG.

# 5 Analytical solutions for the two conceptual models

## 5.1 Mathematical model

The two conceptual models have the same physical settings and only the input and initial conditions change. The mathematical model is based on the following set of assumptions: (i) the system is fully saturated (ii) linear reversible and instantaneous equilibrium partitioning between dissolved and sorbed phases, (iii) mass transport along the fracture is one-dimensional (iv) dispersion along the fracture is neglected, (v) advection in the porous matrix is neglected, (vi) transport in the matrix is perpendicular to the fracture, (vii) degradation can be described as a first-order process and only occurs in the water phase and (viii) separate liquid phase transport is not included.

Under the assumptions described above, the one-dimensional transport equation in a vertical fracture is (Tang et al. 1981):

$$R_f \frac{\partial C_f}{\partial t} + v_f \frac{\partial C_f}{\partial z} + \lambda C_f - \frac{\phi D_m}{b} \frac{\partial C_m}{\partial x} \Big|_{x=b} = 0 \quad (5.1)$$

Where  $C_f$  is the solute aqueous concentration in the fracture ( $M/L^3$ ),  $R_f$  is the retardation coefficient on the fracture surface (-),  $v_f$  is the groundwater velocity in the fracture ( $L/T$ ),  $z$  is the special coordinate along the fracture ( $L$ ),  $b$  is the half aperture of the fracture ( $L$ ) and  $\lambda$  is the first-order degradation rate. The last term represents the mass transfer flux at the fracture-matrix interface ( $M/T/L^2$ ), and depends on the gradient of the aqueous concentration in the matrix  $C_m$  ( $M/L^3$ ), the effective diffusion coefficient  $D_m$  ( $L^2/T$ ), the matrix porosity  $\phi$  and the half fracture aperture.

The transport in the matrix perpendicular to the fracture is described by the one-dimensional diffusion equation:

$$R_m \frac{\partial C_m}{\partial t} - D_m \frac{\partial^2 C_m}{\partial x^2} + \lambda C_m = 0 \quad (5.2)$$

Where  $R_m$  is the retardation factor due to sorption in the matrix.

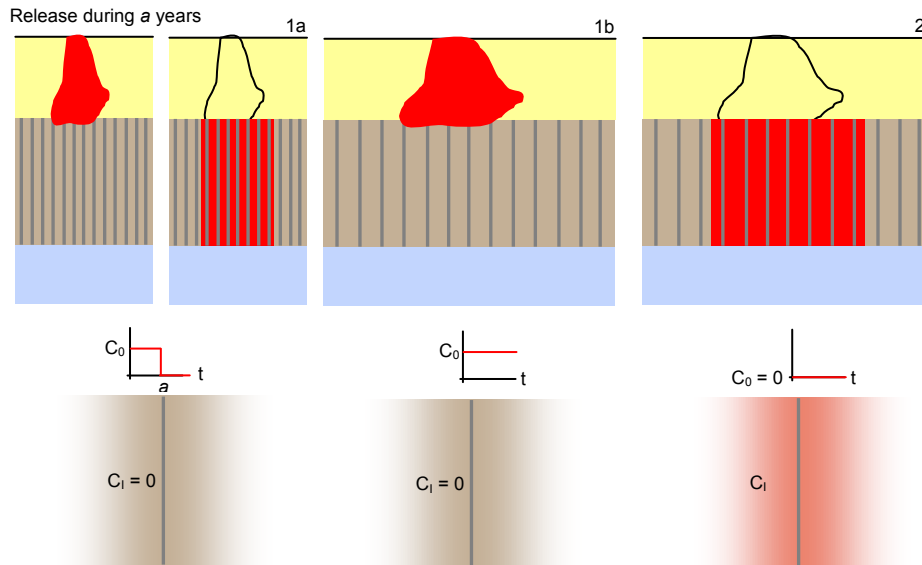


Figure 8 – Conceptual sketch of the three models (top) and the corresponding mathematical boundary and initial conditions (bottom)

## 5.2 Analytical solutions

The analytical solutions are developed from Eq. (5.1) and (5.2) with different initial and boundary conditions illustrated in Figure 8, using the Laplace transform. The details of the development can be found in Appendix A.

### 5.2.1 Model 1

Scenario 1a shown in Figure 8 can be modeled using:

$$A = \frac{bR_f}{\phi\sqrt{R_mD_m}}$$

$$H = \frac{R_f z}{v_f}$$

$$W = \frac{H}{A} + \sqrt{R_m/D_m} (x - b)$$

$$T' = \sqrt{t - H}$$

$$T'' = \sqrt{t - a - H}$$

$$\begin{aligned}
\frac{C_f}{C_0} = \begin{cases} 0 & T' < 0 \\ \frac{1}{2} \exp\left(-\frac{\lambda z}{v_f}\right) \left[ \exp\left(-\frac{H}{A} \sqrt{\lambda/R_m}\right) \operatorname{erfc}\left(\frac{H}{2AT'} - \sqrt{\lambda/R_m} T'\right) + \exp\left(\frac{H}{A} \sqrt{\lambda/R_m}\right) \operatorname{erfc}\left(\frac{H}{2AT'} + \sqrt{\lambda/R_m} T'\right) \right] & T' > 0 \text{ and } T'' < 0 \\ \frac{1}{2} \exp\left(-\frac{\lambda z}{v_f}\right) \left[ \exp\left(-\frac{H}{A} \sqrt{\lambda/R_m}\right) \operatorname{erfc}\left(\frac{H}{2AT'} - \sqrt{\lambda/R_m} T'\right) + \exp\left(\frac{H}{A} \sqrt{\lambda/R_m}\right) \operatorname{erfc}\left(\frac{H}{2AT'} + \sqrt{\lambda/R_m} T'\right) - \exp\left(-\frac{H}{A} \sqrt{\lambda/R_m}\right) \operatorname{erfc}\left(\frac{H}{2AT''} - \sqrt{\lambda/R_m} T''\right) - \exp\left(\frac{H}{A} \sqrt{\lambda/R_m}\right) \operatorname{erfc}\left(\frac{H}{2AT''} + \sqrt{\lambda/R_m} T''\right) \right] & T'' > 0 \end{cases} \\
\\
\frac{C_m}{C_0} = \begin{cases} 0 & T' < 0 \\ \frac{1}{2} \exp\left(-\frac{\lambda z}{v_f}\right) \left[ \exp\left(-W \sqrt{\lambda/R_m}\right) \operatorname{erfc}\left(\frac{W}{2T'} - \sqrt{\lambda/R_m} T'\right) + \exp\left(W \sqrt{\lambda/R_m}\right) \operatorname{erfc}\left(\frac{W}{2T'} + \sqrt{\lambda/R_m} T'\right) \right] & T' > 0 \text{ and } T'' < 0 \\ \frac{1}{2} \exp\left(-\frac{\lambda z}{v_f}\right) \left[ \exp\left(-W \sqrt{\lambda/R_m}\right) \operatorname{erfc}\left(\frac{W}{2T'} - \sqrt{\lambda/R_m} T'\right) + \exp\left(W \sqrt{\lambda/R_m}\right) \operatorname{erfc}\left(\frac{W}{2T'} + \sqrt{\lambda/R_m} T'\right) - \exp\left(-W \sqrt{\lambda/R_m}\right) \operatorname{erfc}\left(\frac{W}{2T''} - \sqrt{\lambda/R_m} T''\right) - \exp\left(W \sqrt{\lambda/R_m}\right) \operatorname{erfc}\left(\frac{W}{2T''} + \sqrt{\lambda/R_m} T''\right) \right] & T'' > 0 \end{cases}
\end{aligned}$$

For model 1b in Figure 8, the solution reduces to the two first terms, for large  $T''$  (the source is not removed).

Furthermore a steady-state concentration can be calculated for model 1b:

$$\begin{aligned}
\frac{C_f}{C_0} &= \exp\left(-\frac{\lambda z}{v_f}\right) \exp\left(-\frac{H \sqrt{\lambda/R_m}}{A}\right) \\
\frac{C_m}{C_0} &= \exp\left(-\frac{\lambda z}{v_f}\right) \exp\left(-\sqrt{\lambda/R_m} W\right)
\end{aligned} \tag{5.3}$$



### 5.2.2 Model 2

For model 2 of Figure 8 the solution is given by:

$$\frac{C_f}{C_i} = \begin{cases} \exp\left(-\lambda/R_m t\right) - \left(\exp\left(-\lambda z/v_f\right) \exp\left(-\lambda/R_m T'^2\right) \operatorname{erfc}\left(\frac{H}{2AT'}\right)\right) & T' > 0 \\ \exp\left(-\lambda/R_m t\right) & T' < 0 \end{cases}$$

$$\frac{C_m}{C_i} = \begin{cases} \exp\left(-\lambda/R_m t\right) - \left(\exp\left(-\lambda z/v_f\right) \exp\left(-\lambda/R_m T'^2\right) \operatorname{erfc}\left(\frac{W}{2T'}\right)\right) & T' > 0 \\ \exp\left(-\lambda/R_m t\right) & T' < 0 \end{cases}$$

### 5.2.3 Input parameters

To compute the analytical solutions, the following parameters are necessary:

- Fracture aperture ( $b$ )
- Groundwater velocity in fracture ( $v_f$ )
- Matrix porosity ( $\phi$ )
- Effective diffusion coefficient in matrix ( $D_m$ )
- Retardation factor in matrix and fracture ( $R_m$  and  $R_f$ )
- First-order degradation rate ( $\lambda$ )

For conceptual model 1, the concentration in the overlying source ( $C_o$ ) is also needed, as well as the duration of contaminant leaching before source removal ( $a$ ) in case of model 1a. For conceptual model 2, the average aqueous concentration in the porous matrix ( $C$ ) is necessary.

Guidance on the selection of parameters and their default values is discussed in Chapter 6.

## 5.2.4 Excel sheet - Examples

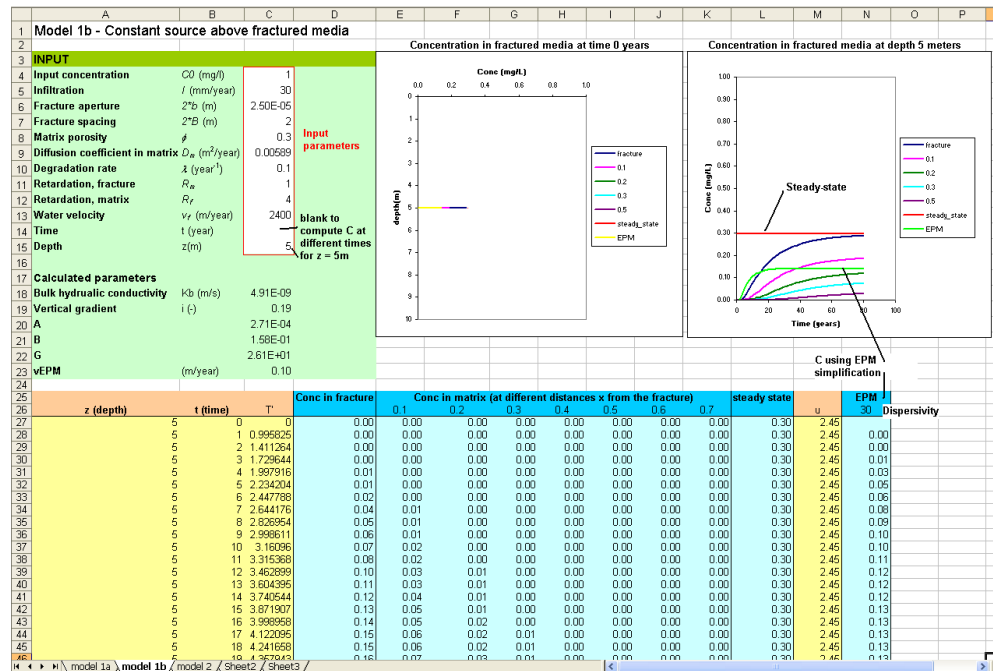


Figure 9 – Excel sheet example for model 1b – solution for varying time at 5 m below the source

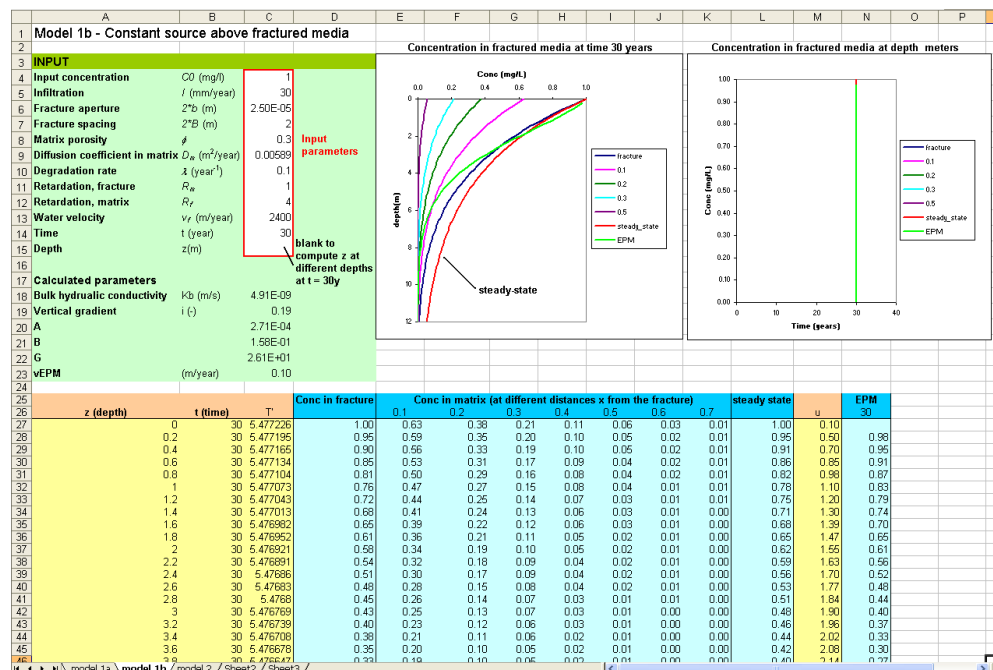


Figure 10 – Excel sheet example for model 1b – solution for varying depth after 30 years of leaching

## 5.3 Model verification

The accuracy of the analytical solutions implemented in Excel is verified by comparing the results with a numerical model developed in Comsol Multiphysics (Chambon et al. 2010). The

results from JAGG2.0 compare well with the numerical model  
(data not shown).

## 6 Choice of parameters

The choice of parameters for transport in fractured media has been extensively discussed and illustrated in SprækkeJAGG (Videncenter for Jordforurening 2008). Therefore it will not be further discussed in this report and the reader is reported to the SprækkeJAGG report for additional information.

### 6.1 Water balance and calculation of water velocity in fracture

#### Fracture velocity based on infiltration

The flow along the fracture in SprækkeJAGG (Videncenter for Jordforurening 2008) is estimated with the following conceptual model: the net precipitation that falls on the land surface will flow downwards through the fractures. Hence the water flow through a single fracture can be estimated with:

$$Q_f = I \cdot 2B \quad (6.1)$$

Where  $Q_f$  is the water flow in the fracture per unit meter ( $L^3/T/L$ ),  $I$  is the net precipitation rate ( $L/T$ ) and  $2B$  is the distance between two fracture ( $L$ ). Based on this approach, the fracture velocity,  $v_f$ , can be calculated:

$$v_f = \frac{Q_f}{2b} = I \cdot \frac{B}{b} \quad (6.2)$$

Where  $2b$  is the fracture aperture ( $L$ ).

In this approach, the flow in the fracture  $Q_f$  does not depend on its aperture. This can lead to unrealistic results when the fracture spacing  $2B$  is large and the aperture  $2b$  is small because in these cases  $Q_f$  and  $v_f$  are very large.

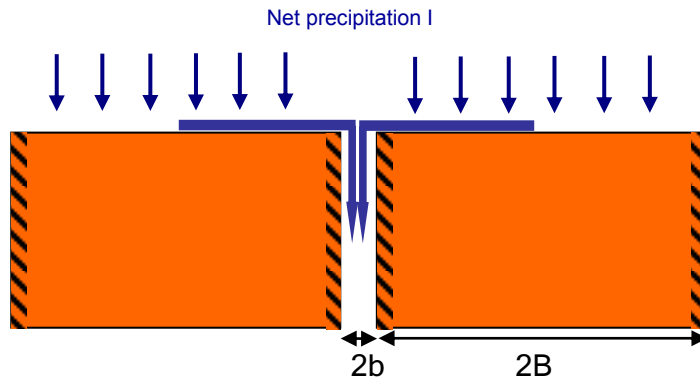


Figure 11 – Definition of flow into fracture in SprækkeJAGG

### Fracture velocity based on “Cubic law” approach

As noted in Miljøstyrelsen (2007), there is another way of defining the water flow through a fracture, where the water flow along a fracture is defined by the hydraulic gradient, hydraulic conductivity and fracture aperture and is a function of the fracture aperture cubed:

$$Q_f = K_f \cdot 2b \cdot i \quad (6.3)$$

Where  $i$  is the vertical hydraulic gradient along the fracture and  $K_f$  is the hydraulic conductivity of the fracture:

$$K_f = \frac{\rho g}{12\mu} (2b)^2 \quad (6.4)$$

Where  $\rho$  is the fluid density ( $M/L^3$ ),  $g$  is the gravitational acceleration ( $L/T^2$ ) and  $\mu$  is the viscosity ( $M/L/T^2$ ).

For fractured media it is common to represent the system using one equivalent porous media model where the fracture matrix system is replaced by an effective homogeneous medium with the overall water conducting properties as the physical system. In this case  $Q_f = 2B \cdot K_b \cdot i$  where for a system of parallel fractures, the bulk hydraulic conductivity of the system  $K_b$  can be determined to be (Mckay et al. 1993):

$$K_b = \frac{2b}{2B} K_f + K_m \quad (6.5)$$

Where  $K_m$  is the hydraulic conductivity of the unfractured clay ( $L/T$ ).

If  $K_m \ll K_b$ , the equation can be reduced to:

$$K_b = \frac{2b}{2B} K_f = \frac{(2b)^3}{2B} \frac{\rho g}{12\mu} \quad (6.6)$$

The bulk hydraulic conductivity can be measured at a field site with slug tests and given an estimation of the fracture spacing, the average hydraulic fracture aperture can be calculated with:

$$(2b)^3 = 2B \frac{12\mu}{\rho g} K_b \quad (6.7)$$

Inserting (6.6) in (6.3) gives:

$$Q_f = 2B \cdot K_b \cdot i \quad (6.8)$$

The equation above has a similar form as Eq. (6.1), where  $I$  is replaced by  $K_b \cdot i$ . The same is valid for the expression of the velocity in the fracture:

$$v_f = \frac{Q_f}{2b} = \frac{2B \cdot K_b \cdot i}{2b} \quad (6.9)$$

The two approaches shown in Eq. (6.2) and (6.9) are valid and equivalent as long as both matrix and fractures are fully saturated and that the hydraulic conductivity of the matrix is very low (Miljøstyrelsen 2007).

From a practical point of view, the input parameters should be constrained so the water balance for the fractured system gives realistic gradient and bulk hydraulic conductivity values. The input values for infiltration rate, fracture spacing and aperture are used to calculate the corresponding bulk hydraulic conductivity and vertical gradient. These values should be in a realistic range for typical low-permeability fractured deposits in Denmark. In JAGG2.0, a “flag” is implemented to indicate values outside the predefined range.



## 7 Application of tool to experimental columns and field data

In order to validate the developed fracture module for JAGG2.0, it is applied to several scientific examples. These examples are well controlled column and field experiments involving conservative and sorbing tracer transport through low-permeability fractured media.

### 7.1 Data overview

Section	Type	Compounds	Duration	Reference	Comments
7.2	Column	Cl <sup>-</sup> and MCP	5 - 300 h	(Jørgensen et al. 1998)	
7.3	Column	Cl <sup>-</sup> and viruses	12 - 80 h	(Hinsby et al. 1996)	
7.4	Field	Br <sup>-</sup> and MCP	35 - 50 days	(Jørgensen et al. 2002)	2 m saturated clay till
7.5	Field	Cl <sup>-</sup> , DBA and dyes	200 h	(Mortensen et al. 2004)	3 m unsaturated clay till
7.6	Field	Br <sup>-</sup>	4.5 years	(Harrar et al. 2007)	8 m saturated clay till

Table 1 – Summary of examples considered in Chapter 7

### 7.2 Column experiments with chloride and pesticides

Undisturbed columns of fractured clayey till were used for tracer experiments with chloride and the pesticide MCP (Jørgensen et al. 1998). Chloride is a conservative tracer, while MCP can sorb on the clay matrix. Both tracers were injected in steady-state water flows through three columns with sediments of different depths. The three columns are characterized by different fracture systems (spacing and aperture).

JAGG2.0 is used to simulate the breakthrough curves of the two compounds for the three columns. The input parameters



are given in Table 2, and the simulated curves are plotted with the measured concentration in Figure 12. JAGG2.0 simulates well the breakthrough curves obtained from column experiments, both for conservative and sorbing tracers.

		Column 1		Column 2		Column 3	
INPUT		Cl <sup>-</sup>	MCP	Cl <sup>-</sup>	MCP	Cl <sup>-</sup>	MCP
Input concentration	C0 (mg/l)	1	1	1	1	1	1
Fracture aperture	2*b (m)	8.40E-05	8.40E-05	8.20E-05	8.20E-05	4.20E-05	2.70E-05
Fracture spacing	2*B (m)	0.025	0.025	0.1	0.1	0.16	0.16
Matrix porosity	φ	0.31	0.31	0.31	0.31	0.31	0.31
Diffusion coefficient in matrix	D* (m <sup>2</sup> /year)	2.16E-06	3.49E-07	2.16E-06	3.49E-07	2.16E-06	3.49E-07
Degradation rate	λ (year <sup>-1</sup> )	0	0	0	0	0	0
Retardation, fracture	R	1	4	1	6.8	1	6.8
Retardation, matrix	R'	1	4	1	6.8	1	6.8
Water velocity	v (m/år)	8.0	8.0	7.6	7.6	4.0	1.7
Spill time	a (year)	4.4	0.6	4.4	1.3	89.0	47.8
Time	t (year)						
Depth	z(m)	0.5	0.5	0.5	0.5	0.5	0.5
<b>Calculated parameters</b>							
Bulk hydraulic conductivity	Kb (m/s)	2.98E-05	2.98E-05	6.93E-06	6.93E-06	2.91E-07	7.74E-08
Vertical gradient	i (-)	1	1	1	1	1	1

Table 2 – Input parameters for simulation of the columns experiments from (Jørgensen et al. 1998)

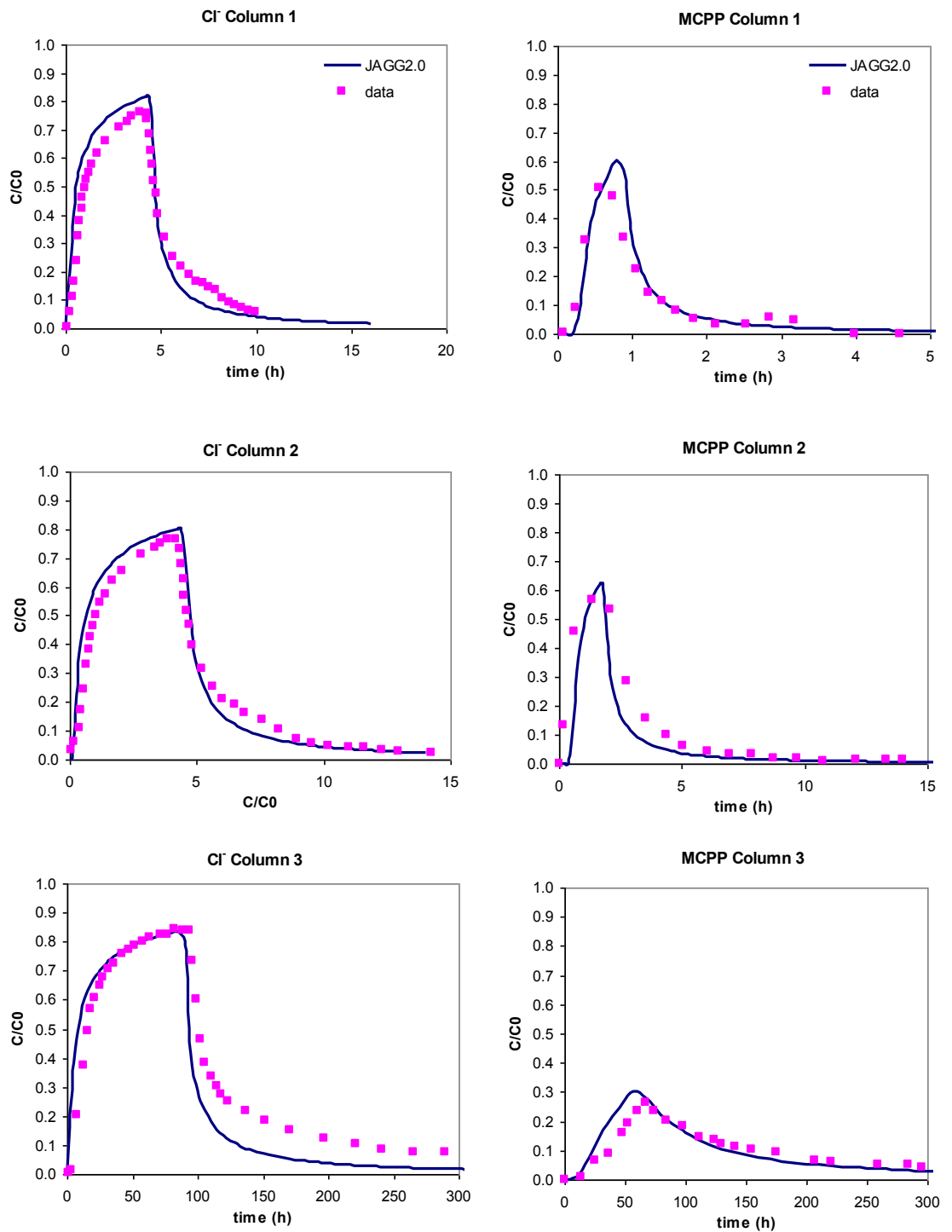


Figure 12 – Simulated and measured breakthrough curves for chloride and MCPP. Data from (Jørgensen et al. 1998)

### 7.3 Column experiments with chloride and bacteriophages

An undisturbed column of fractured clayey till was used for tracer experiments using chloride and two bacteriophages (PRD-1 and MS-2) (Hinsby et al. 1996). Chloride is a solute, while PRD-1 and MS-2 are colloidal tracers that were chosen because their transport is similar to virus (diameter of  $0.062 \mu\text{m}$  and  $0.026 \mu\text{m}$  respectively). The colloidal tracers were

expected to diffuse less into the matrix than chloride due to their larger diameters. The three tracers were injected at steady-state water flows through the column. The three columns were characterized by different fracture systems (spacing and aperture).

JAGG2.0 is used to simulate the breakthrough curves of the three compounds for the two experiments. The input parameters are shown in Table 3, and the simulated curves are plotted with the measured concentration in Figure 13. JAGG2.0 simulates well the breakthrough curves obtained for chloride. However the calibrated diffusion coefficient is the same for the three tracers despite the fact that the coefficients for the bacteriophage were expected to be lower than for chloride due to their larger size. Furthermore the experimentally observed breakthrough curves for bacteriophages show a much smaller steady-state concentration than the input concentration. This attenuation can be fitted with a first-order degradation rate, but this process is not likely representative, as the attenuation is probably due to filtration in the fractures and to electrostatic or hydrophobic attraction to mineral or organic surfaces in the soil (Hinsby et al. 1996).

		Exp 2		Exp 3
INPUT		PRD	MS	CI'
Input concentration	C0 (mg/l)	200000000	1800	1
Fracture aperture	2*b (m)	5.80E-05	5.80E-05	5.80E-05
Fracture spacing	2*B (m)	0.22	0.22	0.22
Matrix porosity	$\phi$	0.3	0.3	0.3
Diffusion coefficient in matrix	D' (m <sup>2</sup> /year)	2.16E-06	2.16E-06	2.16E-06
Degradation rate	$\lambda$ (year <sup>-1</sup> )	0 - 0.5	0 - 1	0
Retardation, fracture	R	1	1	1
Retardation, matrix	R'	1	1	1
Water velocity	v (m/år)	3.4	3.4	3.4
Spill time	a (year)	43.0	43.0	43.0
Time	t (year)			
Depth	z(m)	0.5	0.5	0.5
<b>Calculated parameters</b>				
Bulk hydraulic conductivity	Kb (m/s)	1.12E-06	1.12E-06	1.12E-06
Vertical gradient	i (-)	0.45	0.45	0.45

Table 3 – Input parameters for simulation of column experiments from (Hinsby et al. 1996)

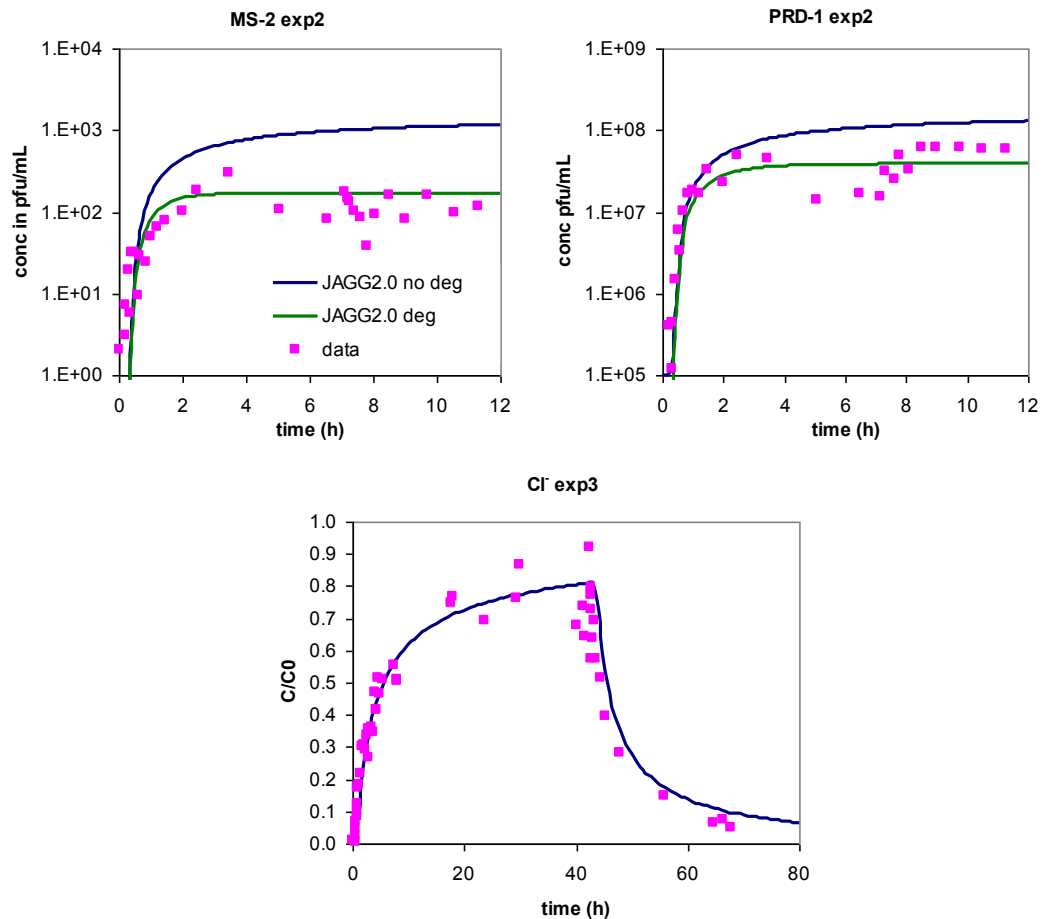


Figure 13 – Simulated and measured (pink markers) breakthrough curves. The blue curves show the model results without degradation while the green curve shows the model with a fitted degradation rate. Data from (Hinsby et al. 1996)

From these experiments, it can be concluded that JAGG2.0 does predict the fast breakthrough of colloids but the steady-state concentration is overestimated if attenuation by filtration/attraction is not taken into account.

#### 7.4 Field experiments in saturated fractured clayey till

Bromide and MCPP were infiltrated through a 2 meter deep water saturated clayey till and the concentrations in the underlying sand layer was monitored by Jørgensen et al. (2002). Again bromide is a conservative tracer, while MCPP can sorb on the clay matrix. The breakthrough curves in the underlying sand aquifer are simulated by coupling JAGG2.0 and a one-dimensional porous media equation for the sand layer. The analytical solution for the one-dimensional advection-dispersion equation is given in van Genuchten and Alves (1982 p.31). The results in Figure 14 show a fairly good fit between the measured and simulated concentrations both in term of peak concentration and arrival time.

INPUT		Br <sup>-</sup>	MCPP
Input concentration	C <sub>0</sub> (mg/l)	1	1
Fracture aperture	2*b (m)	3.50E-05	3.50E-05
Fracture spacing	2*B (m)	5.17	5.17
Matrix porosity	φ	0.25	0.25
Diffusion coefficient in matrix	D <sub>m</sub> (m <sup>2</sup> /day)	4.23E-05	8.42E-06
Degradation rate	λ (day <sup>-1</sup> )	0	0
Retardation, fracture	R	1	6.8
Retardation, matrix	R <sub>m</sub>	1	6.8
Water velocity	v <sub>f</sub> (m/day)	53.2	53.2
Spill time	a (day)	11.7	11.7
Time	t (dat)		
Depth	z(m)	1.7	1.7
Pore Velocity in aquifer	v <sub>aq</sub> (m/day)	2.4	2.4
Longitudinal dispersivity	α (m)	1.2	1.2
Aquifer thickness	h (m)	0.5	0.5
<b>Calculated parameters</b>			
Bulk hydraulic conductivity	K <sub>b</sub> (m/s)	1.04E-08	1.04E-08
Vertical gradient	i (-)	0.8000	0.8000

Table 4 – Input parameters for simulation of field experiments from (Jørgensen et al. 2002)

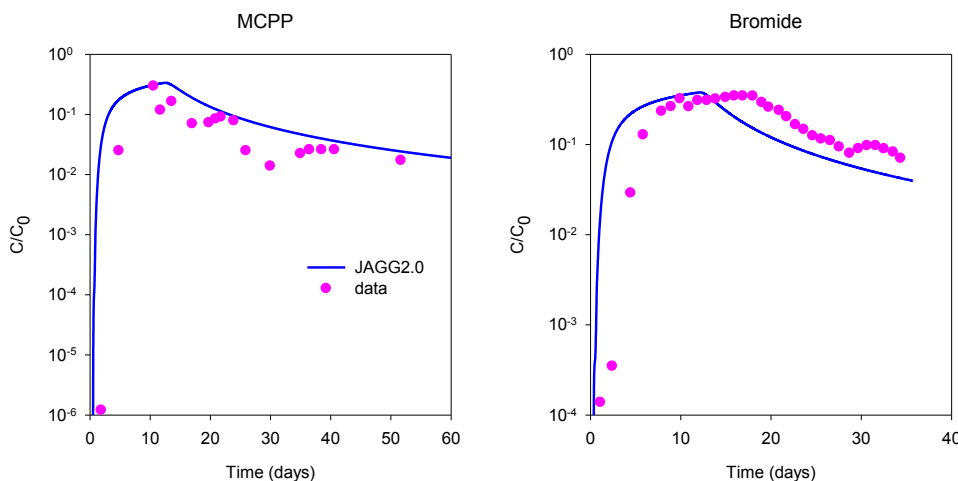


Figure 14 – Simulated and measured concentration in the sand layer underlying the fractured clayey till. Data from (Jørgensen et al. 2002)

This experimental data shows that JAGG2.0 can be used to simulate the fast breakthrough (due to fractures) and the tailing (due to matrix diffusion), using reasonable parameter values.

An EPM (equivalent porous media) model can be compared with JAGG2.0 for this example. With an EPM model, the breakthrough and the tailing are controlled by the choice of the porosity and dispersivity values. In Figure 15 unrealistic values for porosity and/or dispersivity have to be used to correctly simulate the MCPP breakthrough curves. A model that accounts explicitly for transport in fractures, such as JAGG2.0, is thus necessary to describe the flow and transport in fractured media.

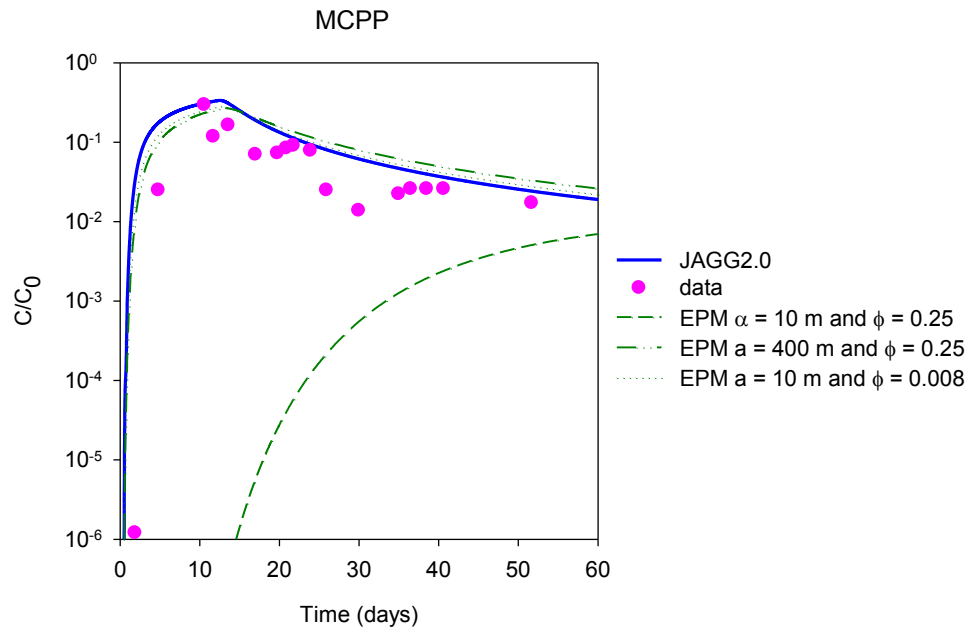


Figure 15 – MCPP breakthrough fitted with EPM model

### 7.5 Field experiments in unsaturated fractured clayey till

In the experiments performed by Mortensen et al. (2004), tracers were infiltrated through a 3 meter deep unsaturated fractured clayey till, under different steady-state flow conditions. The tracers were chloride, DBA and fluorescence dyes. Chloride and DBA are conservative tracers, while fluorescence dyes can sorb on the clay matrix. While the fracture module JAGG2.0 is intended for saturated porous media, it can be applied to this experiment because the matrix was expected to be fully saturated, and only preferential flowpaths like fractures and macropores were unsaturated (Mortensen et al. 2004).

		6.2 mm/h			9.6 mm/h		
INPUT		Cl <sup>-</sup>	2,3-DFBA	Sulfo. B	Cl <sup>-</sup>	2,6-DFBA	Uranine
Input concentration	C0 (mg/l)	1	1	1	1	1	1
Infiltration	I (mm/h)	6.2	6.2	6.2	9.6	9.6	9.6
Fracture aperture	2 <sup>a</sup> b (m)	1E-05	1E-05	1E-05	1E-05	1E-05	1E-05
Fracture spacing	2 <sup>a</sup> B (m)	0.07	0.07	0.07	0.04	0.04	0.04
Matrix porosity	φ	0.25	0.25	0.25	0.25	0.25	0.25
Diffusion coefficient in matrix	D <sub>m</sub> (m <sup>2</sup> /h)	9.9E-07	7.3E-07	2.8E-07	9.9E-07	7.3E-07	4.0E-07
Degradation rate	λ (h <sup>-1</sup> )	0	0	0	0	0	0
Retardation, fracture	R	1	1	1	1	1	1
Retardation, matrix	R <sub>m</sub>	1	1	5	1	1	2
Water velocity	v <sub>f</sub> (m/h)	43.4	43.4	43.4	38.4	38.4	38.4
Spill time	a (h)	2	2	0.40	0.1	0.1	0.05
Time	t (h)						
Depth	z(m)	3	3	3	3	3	3

Table 5 – Input parameters for simulation of experiments from (Mortensen et al. 2004)

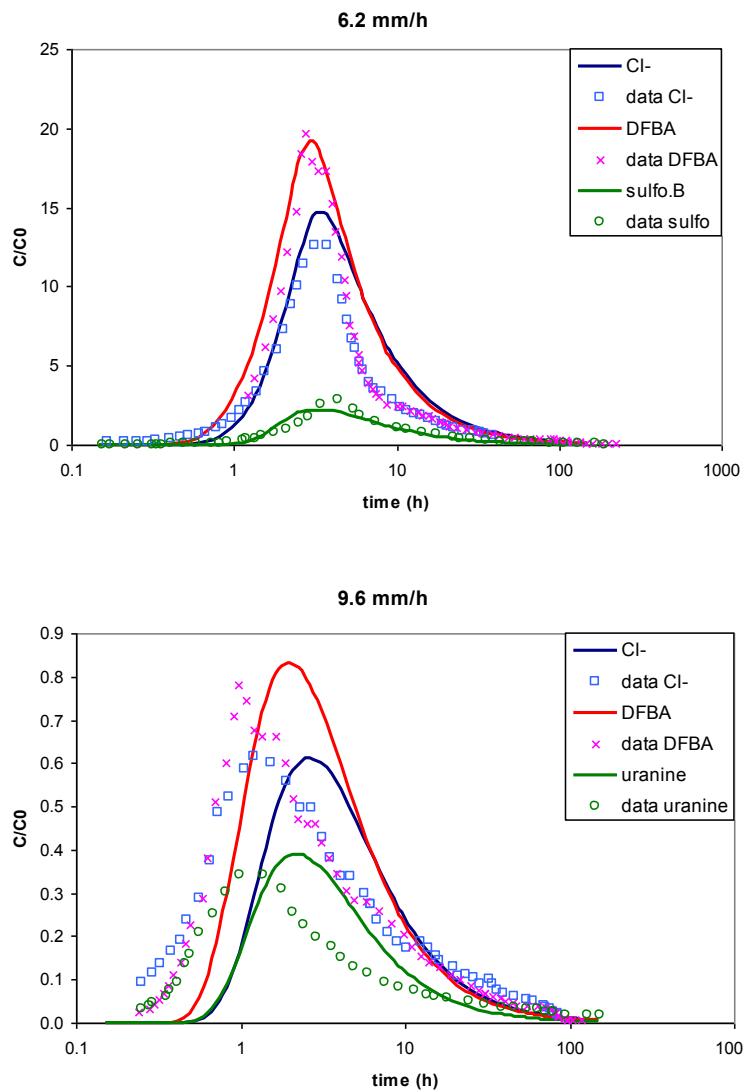


Figure 16 – Simulated and measured breakthrough curves for two steady-state water flows. Data from (Mortensen et al. 2004)

The breakthrough curves are shown in Figure 16 and are well simulated for the experiment at 6.2 mm/h, with an attenuated peak concentration of chloride compared to DFBA due to higher diffusion into the matrix and a low peak concentration of the fluorescence dye (sulfo. B) due to sorption in the clay matrix (retardation coefficient  $R = 5$ ). The peak of the breakthrough curves for the experiments at 9.6 mm/h are well simulated, but the breakthrough time is delayed compared to the observed data. Furthermore it was necessary to decrease the fracture spacing value compared to the calibrated data of the previous experiment (at 6.2 mm/h) to obtain this reasonable fit. This can be explained by the fact that more fractures become saturated and hence hydraulically active under the higher water flow. The relative breakthrough curves of the three compounds are well characterized with attenuation of chloride (due to higher diffusion) and uranine (due to sorption) compared to DFBA.

These experiments illustrate the limitations of applying the fracture module JAGG2.0 to unsaturated conditions, where the amount of hydraulically active fractures varies depending on water flow through the fractured system.

#### 7.6 Long-term field experiment in fractured clay – Bromide injection

A long-term field experiment has been performed at Flakkebjerg (Harrar et al. 2007). Bromide was injected over a period of 22 days with a concentration of 10000 mg/L through an infiltration basin of 2\*2 meters located 2 meters below surface. Tracer infiltration was performed under enhanced flow with an average infiltration rate of 34 mm/d. With these rates it can be seen that 30 kg of bromide was injected in the till. Water infiltration without bromide was maintained at the high rate of 12 mm/day for 158 days after bromide injection. The rest of the experiment was conducted under natural flow conditions where the infiltration rate was estimated to be 0.7 mm/day. The bromide concentration was monitored for 4.5 years by sidewall samplers located in the till at intervals between the bottom of the infiltration basin (2 mbs) and the aquifer 11 meters below surface. The resulting breakthrough curves for monitoring points located at 2, 3.5, 4 and 5.5 mbs are shown in Figure 17. It can be seen that the concentration just below the infiltration basin (2mbs) decreases slowly from a relative concentration of 70% to 0.1% after 1500 days (4 years). Although bromide was injected for only 22 days, a long-term source with decreasing concentration formed just below the infiltration basin. The bromide front reaches 4mbs after 180 days and the concentration at this depth remains constant at 10% of the initial values for the whole monitoring period. The concentration at 4mbs is higher than that measured at 3.5 mbs for the whole monitoring period. This can be due to the fact that a reduced till with a lower hydraulic conductivity is present between 4 and 11 mbs, leading to accumulation of the bromide at the top of this reduced zone (Harrar et al. 2007). This explanation seems to be confirmed by the breakthrough curve at 5.5 mbs, which has a different shape, with increasing concentration up to 2% after 1730 days (4.5 years).

The presence of zones with different hydraulic properties in the till makes the use of a simple model difficult. In the fracture module JAGG2.0, the properties are assumed to be uniform throughout the till. Furthermore with the simple model, it is not



possible to take into account the different infiltration rates employed during the experiment.

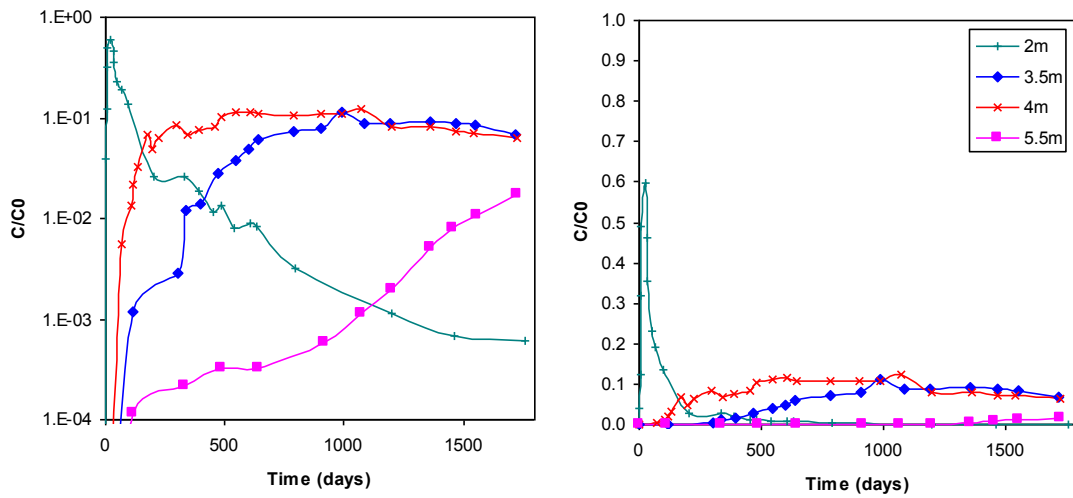


Figure 17 - Breakthrough curves as a function of time and depth in log-scale (left) and normal scale (right). Adapted from (Harrar et al. 2007)

Considering the complexity of the infiltration rate and flow velocity in the system, two approaches are used for modeling this dataset with JAGG-2 and with an EPM:

- Modeling 22-days of bromide infiltration with infiltration rate of 34 mm/day
- Modeling the bromide injection using the natural flow rate (0.7 mm/day) for 1070 days (to obtain the injection of the same total mass of bromide)

The parameters for JAGG2.0 (fracture spacing, aperture and porosity) are adjusted to fit the data and obtain reasonable values for the bulk hydraulic conductivity and the hydraulic gradient under natural flow conditions. The parameters are summarized in Table 6.

The results of JAGG2.0 and the corresponding EPM model are shown in Figure 18 and Figure 19 for the two approaches described above.

INPUT			
Input concentration	C0 (mg/l)	1	1
Infiltration	I (mm/d)	34	0.7
Fracture aperture	2*b (m)	2.2E-05	2.2E-05
Fracture spacing	2*B (m)	0.3	0.3
Matrix porosity	$\phi$	0.3	0.3
Diffusion coefficient in matrix	D' (m <sup>2</sup> /d)	5.1E-05	5.1E-05
Degradation rate	$\lambda$ (år <sup>-1</sup> )	0	0
Retardation, fracture	R	1	1
Retardation, matrix	R'	1	1
Water velocity	v (m/d)	464	10
Spill time	a (d)	22	1070
Time	t (d)		
Calculated parameters			
Bulk hydraulic conductivity	Kb (m/s)	2.23E-08	2.23E-08
Vertical gradient	i (-)	17.63	0.36

Table 6 – Input parameters for Flakkebjerg Bromide injection

For the case of 22-days infiltration under enhanced flow conditions (Figure 18), the two models fail at simulate the data; the breakthrough curves at 3.5, 4 and 5.5 mbs reach 80-90% of the injected concentration within few days, whereas the breakthroughs at these depths were first measured after 100 days (Figure 17). This means that the water injected in the infiltration basin does not flow at the enhanced rate of 34 mm/day throughout the till. As explained previously, it is probable that the infiltrated water containing bromide remains below the infiltration basin and forms a long term source for the underlying fractured till.

For the case of 1070-days infiltration under natural flow conditions (Figure 19) it is not possible to simulate the data either. It is possible that some of the injected bromide has flown horizontally, far from the monitoring samplers. Furthermore the assumption of a one-dimensional vertical transport may not be valid, given the small size of the infiltration basin ( $2 \times 2 \text{ m}^2$ ). Therefore a more complex model would be necessary to take into account the processes affecting vertical transport of bromide

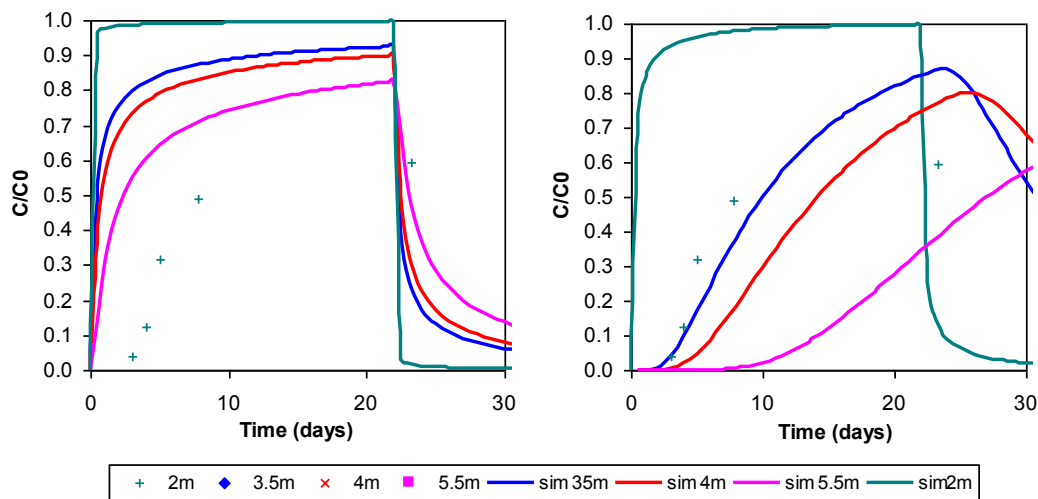


Figure 18 - Fracture JAGG-2 (left) and EPM model (right) for a 22-days pulse source under enhanced flow rate (37 mm/day). Data from (Harrar et al. 2007)

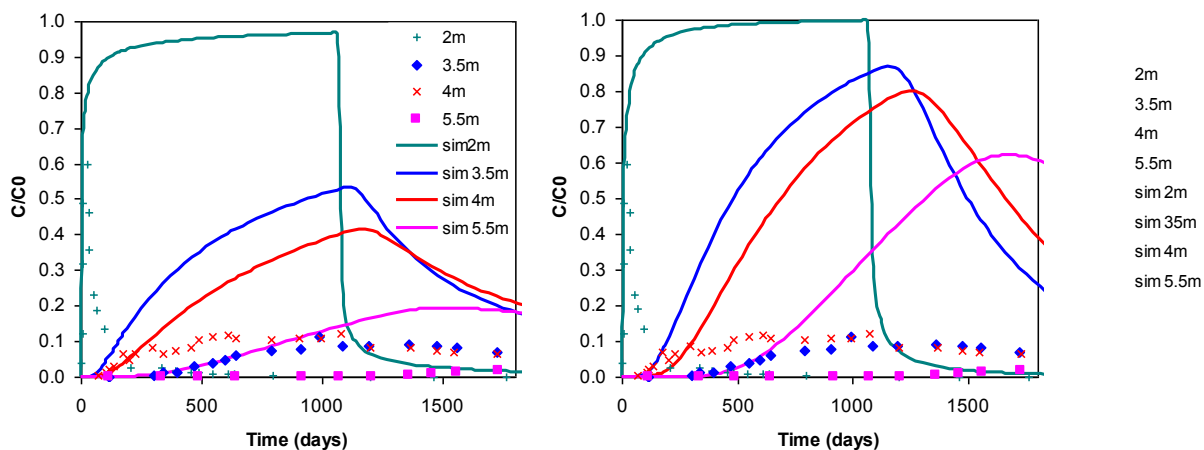


Figure 19 - Fracture JAGG-2 (left) and EPM model (right) for a 1070-days pulse source under natural flow rate (0.7 mm/day). Data from (Harrar et al. 2007)

It seems that the assumption of uniform flow velocity throughout the till is not valid and that differences in hydraulic conductivities are controlling bromide transport at Flakkebjerg. However the breakthrough curves present the typical shape of fast breakthrough and long tailing. Bromide infiltration lasted for only 22 days, but high concentrations (0.1 and 10%) are measured in the till at several depths more than 4 years after.

This long tailing can be explained by slow back diffusion from the matrix to the fracture system, or by slow vertical advection-dispersion through the porous media.

#### 7.7 Validity of JAGG2.0

The examples described in this chapter show that JAGG2.0 simulates well the results of experiments performed both on clayey till columns and in the field. JAGG2.0 can describe the fast contaminant breakthroughs and long tailings characterizing flow and transport in fractured clay systems. Sorption processes are simulated well and the differences between the contaminants are well described (conservative vs. sorbing compounds). However we did not find experimental data where degradation takes place. These experiments verify the conceptual model of fast transport through the fractures and slow diffusion into the matrix.

Furthermore the use of a model which explicitly accounts for flow along fractures (such as JAGG2.0), is necessary to simulate the experimental results with realistic parameters, as shown by the example in 7.4. An EPM model fitting the data will require the use of unrealistic values for the porosity and/or the dispersivity of the porous media.

However the experiments presented in this chapter (besides Flakkebjerg) are of short duration (maximum of 70 days for the field experiment in 7.4), and have focused on the validation of the conceptual model of fast contaminant breakthrough through fractures and retardation due to diffusion into the matrix. The long term leaching (over years and decades) due to slow back diffusion from the matrix to the fracture system has not been documented, because of the long timeframes. In the context of risk assessment, contamination has often occurred over long time periods and the risk should be assessed years/decades after (see examples with pesticides spreading and chlorinated solvents spill in Chapter 8). The data available from the experiments do not allow the verification of the model for the long term leaching from the contaminated fractured media due to slow back diffusion.



## 8 Case studies for risk assessment

This chapter considers the use of the risk assessment fracture module JAGG2.0 for a set of practical examples similar to those likely to occur in practice. In each case JAGG2.0 output is compared with the observed data for an example published. An overview of the examples and case studies is shown in Table 7.

### 8.1 Overview of case studies

Section	Type	Site	Compounds	Model	Reference
8.2.1	Diffusive source	Hvidovre	Pesticides (DCB and BAM)	1a	(Miljøstyrelsen 2002c)
8.2.2	Point source	Skælskør	Pesticides	1a	(Miljøstyrelsen 2009b)
8.3.1	DNAPL	Sortebrovej	TCE and DCE	1a	(Fyns Amt 2004)
8.3.2	Contam. till	Gl. Kongevej	TCE	2	(Miljøkontrollen 2004b)
8.4	Gas station	Svendborg	MTBE and benzene	1b	(Miljøstyrelsen 2003)

Table 7 – Summary of the case studies considered in chapter 8

### 8.2 Pesticides in groundwater

#### 8.2.1 Diffusive sources of dichlobenil and BAM

JAGG2.0 is applied to assess the risk posed by the use of the pesticide dichlobenil (DCB) to underlying groundwater. This pesticide has been used extensively in Denmark between 1966 and 1997 (Miljøstyrelsen 2002c). DCB is known to degrade to BAM under aerobic conditions in the upper part of the soil (mainly above 3 meters), with a half-life constant around 0.5 year (Miljøstyrelsen 2002c). Below this depth, DCB degradation decreases very fast with increasing depth.

In this study, JAGG2.0 is used to assess the risk posed by the degradation product BAM, resulting from the application of

DCB on treated soils. The system must be simplified before application of JAGG2.0. It is assumed that all DCB applied on the soil is degraded to BAM within the upper three meters of the soil. This assumption is justified by the fact that DCB is rarely found below 3 meters (Miljøstyrelsen 2002a). JAGG2.0 is then applied to the fractured clayey till from 3 mbs.

For the general case, the applied parameters are shown in Table 8. The input concentration is calculated with the assumption of an effective application of 5kg/ha/year during 30 years (Miljøstyrelsen 2002c). It can also be noted that BAM is modeled as a non-degradable compound, as shown in Miljøstyrelsen (2002b).

INPUT		
Input concentration	$C_0$ ( $\mu\text{g/l}$ )	4605
Infiltration	$I$ (mm/år)	120
Fracture aperture	$2*b$ (m)	$3.00\text{E-}05$
Fracture spacing	$2*B$ (m)	1
Matrix porosity	$\phi$	0.25
Diffusion coefficient in matrix	$D'$ ( $\text{m}^2/\text{år}$ )	0.003548
Degradation rate	$\lambda$ (år $^{-1}$ )	0
Retardation, fracture	$R$	1
Retardation, matrix	$R'$	8.29
Water velocity	$v$ (m/år)	4000
Spill time	$a$ (year)	30

Table 8 – Input parameters for BAM contamination through fractured clayey till

The modeling results assuming a 5 meters deep clayey till (3-8 mbs) are shown in Figure 20. At the fracture outlet, the BAM breakthrough is very fast with a peak concentration of 3000  $\mu\text{g/L}$  followed by a long tailing to concentrations of about 100  $\mu\text{g/L}$ , which last at least until 2100. The pore water concentration in the matrix at a distance of 0.5 m from the fracture reaches 1 $\mu\text{g/L}$  around 1990 and remains below 100  $\mu\text{g/L}$  for the whole period. Water sampled from the monitoring wells in clay till contains both fracture and matrix water and so is expected to show a concentration between these two curves.

The result from an EPM model (with standard values for porosity (0.25) and dispersivity (0.1 m)) is also shown in the figure. The concentration is characterized by a late breakthrough (around 2006), a peak concentration of 3000  $\mu\text{g/L}$  around year 2060, followed by a decrease.

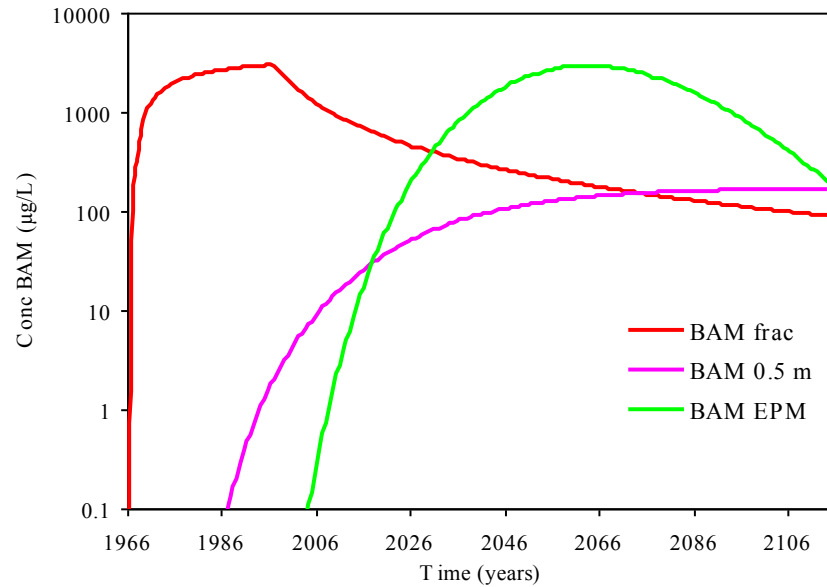


Figure 20 – BAM concentration at the fracture outlet (red) and in the matrix at a distance of 0.5 m from the fracture (pink), under 5 meters of clayey till (8 mbs). The result of an EPM model is also shown in green

These results are very difficult to compare with field data, as no records are available before 1995. However a qualitative comparison can be done, with data from Hvidovre municipality. The site is characterized by a thick clayey till (5-12 meters) overlying a chalk aquifer, where 14 drinking wells pump 800000 m<sup>3</sup>/year (Miljøstyrelsen 2002a). BAM has been detected in several drinking wells and in the clayey till overlying the chalk aquifer. Results from investigations in 2002 are shown in Figure 21. DCB is rarely detected below 3 meters depth, confirming our conceptual model. Furthermore, BAM is found in the clayey till at concentrations between 2-37 µg/L. These concentrations are much higher than the simulated concentration for an EPM model in Figure 20 (<0.1 µg/L until 2005), which seems to confirm the fractured characteristics of the clayey till. However, the concentrations are also much lower than the simulated concentration in the fracture (around 2000 µg/L). They are located between the two curves for the fracture and the matrix at a distance of 0.5 meter. The concentration in a fractured clayey till depends on the distance of the sample point from a hydraulically active fracture. Furthermore other heterogeneities, such as horizontal sand lenses/fractures can also influence measured concentrations.



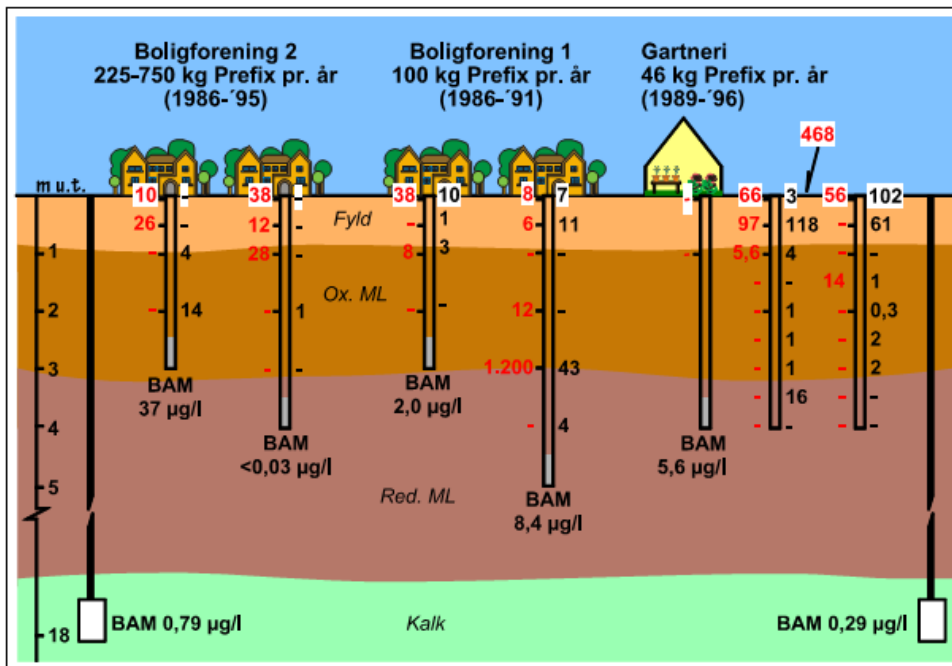


Figure 21 – Dichlobenil (red) and BAM (black) concentration in soil (µg/kg) and porewater (µg/l) in 3 sites in Hvidovre (Miljøstyrelsen 2002a)

The expected BAM concentration in the pumping wells can also be calculated from JAGG2.0 results. Assuming that all the contaminated groundwater is pumped by the 14 wells, the concentration in the wells can be evaluated using Eq.(3.6) and:

$$C_{well} = C_{frac} \cdot \frac{A \cdot I}{800000} \quad (8.1)$$

Where A is the soil area treated with DCB and I is the annual infiltration rate ( $I = 120 \text{ mm/year}$ ). A is not known for Hvidovre, but is estimated based on Miljøstyrelsen (2002c) to be between  $3000 - 16000 \text{ m}^2$ .

The resulting concentration in the pumping wells (assuming a uniform pumping rate among the 14 wells) is shown in Figure 22. The simulated concentrations are above the measured concentrations at the drinking wells, which ranged between 0 and  $0.8 \text{ µg/L}$  (between 1995 and 2008), but the presence of pesticides is well simulated compared to the results with the EPM model, which predicts a BAM breakthrough (above  $0.01 \text{ µg/L}$ ) in the drinking well starting in 2015). BAM and other pesticides have been measured in the drinking water wells as early as 1995, but the actual breakthrough time is unknown and so cannot be compared with the simulated fast breakthrough from the model (few years after starting of BAM application in 1966).

JAGG2.0 simulates the observed BAM concentrations in the drinking wells, and the expected duration of the contaminant impact can be assessed. JAGG2.0 shows that the concentration in the drinking water well is expected to remain above 0.1  $\mu\text{g/L}$  until at least 2050 (for the case of a smaller treated area).

Note that this is a risk assessment model with many simplifications. It is intended for assessment of risk based on few available data. Its use in prediction should be done with great caution.

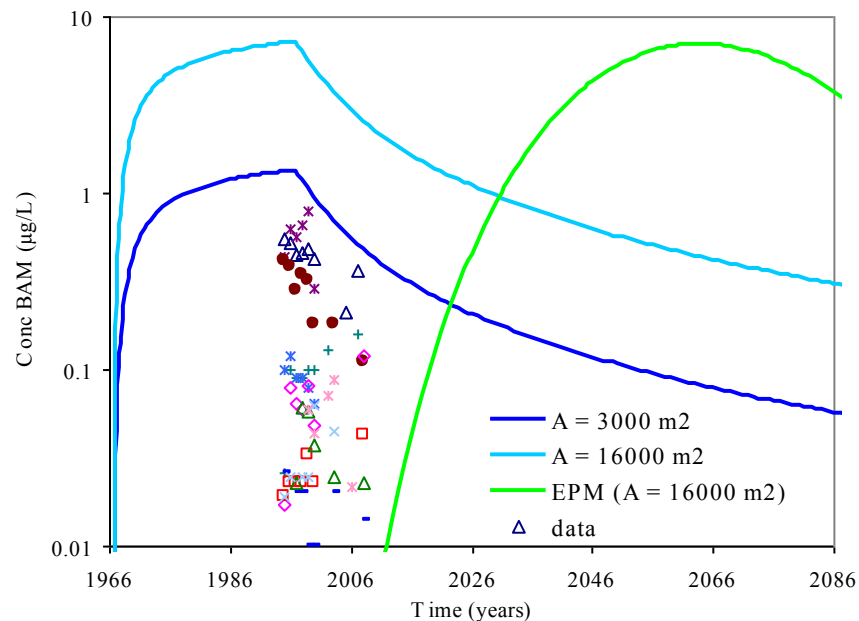


Figure 22 - Simulated concentration at the drinking wells, assuming a treated area of 3000 and 16000  $\text{m}^2$ , with data from 11 drinking wells (overlain by 4 to 7m clayey till) between 1995 - 2008 from Jupiter database

The parameters for the EPM model can be modified so that it simulates the presence of BAM in the drinking wells in 1995-2008, as shown in Figure 23. But the breakthrough time in the drinking wells is unknown, so it is not possible to determine if this model is realistic. The available data therefore cannot be used to validate the fracture module JAGG2.0 model over a simple EPM model.

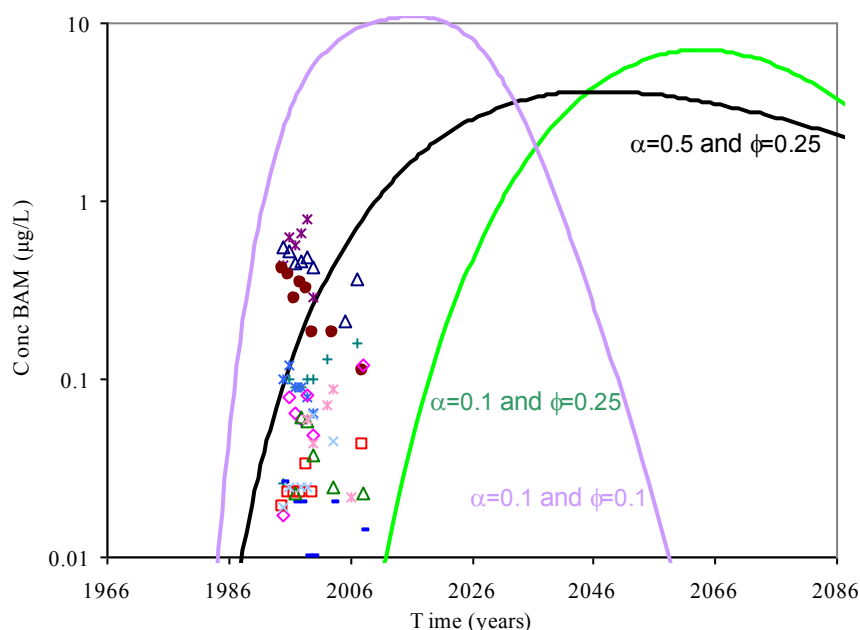


Figure 23 – EPM model with different porosity and dispersivity values. data from 11 drinking wells (overlain by 4 to 7m clayey till) between 1995 – 2008 from Jupiter database

### 8.2.2 Point source of pesticides at Skælskør

Pesticides have been monitored at a point source site near an orchard in Skælskør. In this site, a range of pesticides have been used since the 1960's. Water and soil samples have been analyzed in 93/94 (Miljøkontrollen 2000) and 2007 (Miljøstyrelsen 2009b). Hence this site represents an interesting dataset with two monitoring rounds separated by 15 years. The site is characterized by a 25 meters clay till overlying the regional aquifer. Three boreholes with multilevel samplers in the glacial till down to the level of the underlying aquifer have been installed in 1993 and seven new boreholes were drilled in 2007. Concentration profiles for a range of pesticides in 93/94 and 2007 is presented in Miljøstyrelsen (2009b). In this section, we will focus on dichlorprop, mecoprop (DCPP and MCP) and MCPA occurrence in the clayey till.

The monitoring results in Figure 25 show that the concentration profiles in the till are quite variable. This can be due to the fact that the concentration in a fractured clayey till depends on the distance of the sample point from preferential pathways. Furthermore other heterogeneities, such as sand lenses/fractures can also influence the concentrations. It is also shown that all three pesticides have been detected in the underlying regional aquifer located 25 meters below surface.

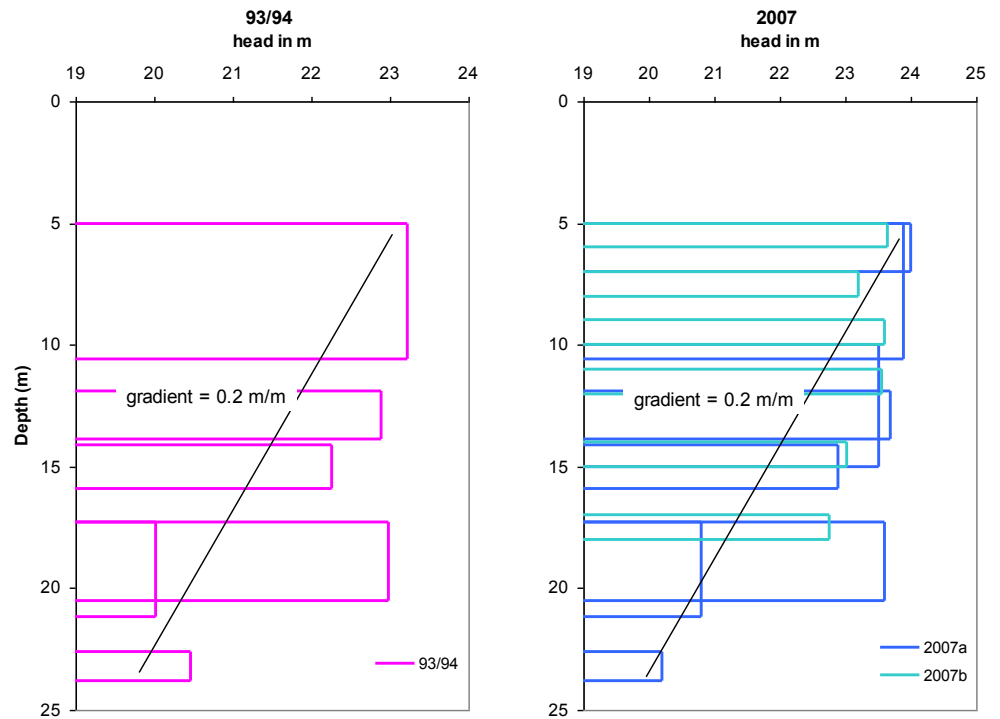


Figure 24 - Head in the glacial till in 93/94 and 2007. Modified from (Miljøstyrelsen 2009b)

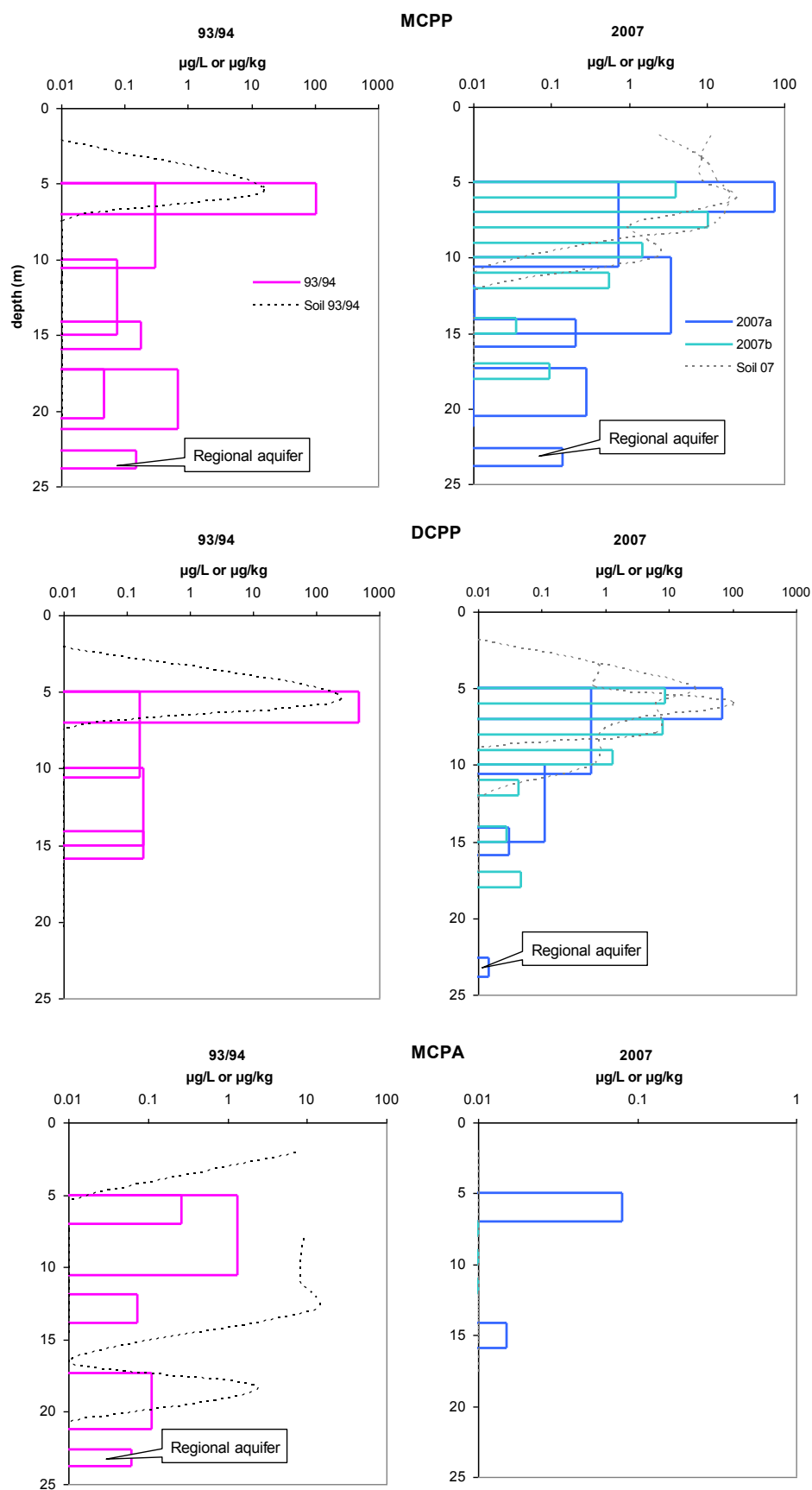


Figure 25 –MCPA, MCPP and DCP concentration throughout the clay till under the point source, modified from (Miljøstyrelsen 2009b)

In this study, JAGG2.0 is used to simulate the concentration profiles of the three pesticides in 93/94 and 2007. The system has to be simplified before application of the model. The upper 4 meters consist of clay fill with different hydraulic properties to the underlying 20 meters clayey till, therefore this layer is not taking into account in JAGG2.0 and the tool is then applied to the fractured clayey till from 4 mbs. The parameters are taken from Miljøstyrelsen (2009b), but some simplifications are needed. For example, the infiltration is taken equal to the groundwater recharge 30 mm/year, whereas in Miljøstyrelsen (2009b) a more complex model is used, which takes into account horizontal flow in interbedded sand layers. The fracture spacing, as well as the matrix porosity are taken directly from Miljøstyrelsen (2009b). The fracture aperture is adjusted to obtain the measured hydraulic gradient (0.2 m/m) and a reasonable bulk hydraulic conductivity. As the matrix is assumed to be impermeable in Miljøstyrelsen (2009b) so that water is flowing through the fractures only, the water velocity in the fractures becomes very high (1500 m/y).

INPUT		DCPP	MCP	MCPA
Input concentration	$C_0$ (mg/l)	10	0.4	0.4
Infiltration	$I$ (mm/year)	30	30	30
Fracture aperture	$2*b$ (m)	2.00E-05	2.00E-05	2.00E-05
Fracture spacing	$2*B$ (m)	1	1	1
Matrix porosity	$\phi$	0.3	0.3	0.3
Diffusion coefficient in matrix	$D_m$ (m <sup>2</sup> /year)	0.0039	0.0039	0.0039
Degradation rate	$\lambda$ (year <sup>-1</sup> )	0.30	0	2.77
Retardation, fracture	$R_f$	1	1	1
Retardation, matrix	$R_m$	2	2	6.8
Water velocity	$v_f$ (m/year)	1500	1500	1500
Spill time	$a$ (year)	24	24	24
Bulk hydraulic conductivity	$K_b$ (m/s)	5.0E-09	5.0E-09	5.0E-09
Vertical gradient	$i$ (-)	0.19	0.19	0.19
Average velocity in EPM	$v_{EPM}$ (m/year)	0.1	0.1	0.1

Table 9 – Input parameters for point source of pesticides in Skælsør

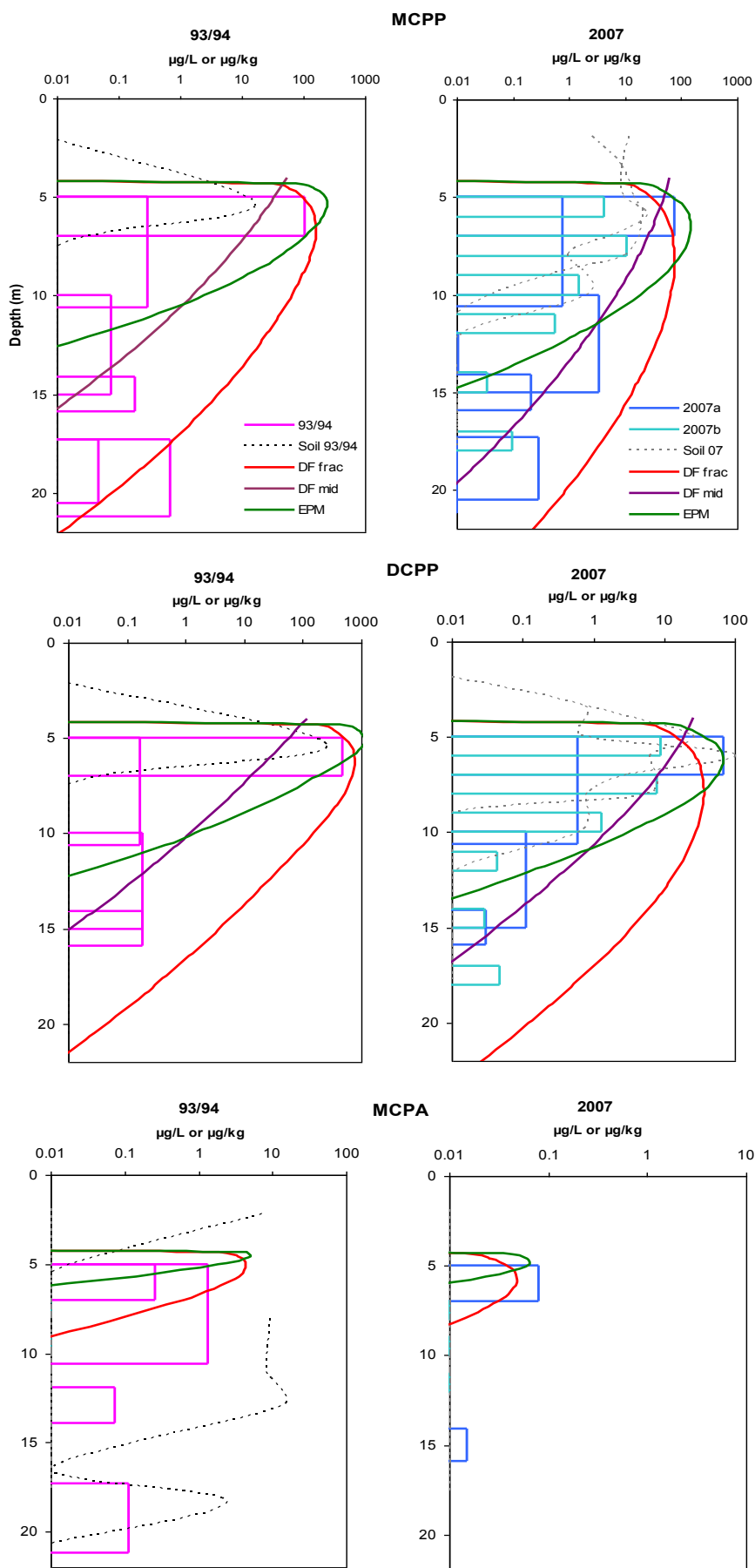


Figure 26 – Measured and simulated concentrations along the till in 93/94 (top) and 2007 (bottom). Data from (Miljøstyrelsen 2009b)

The results from JAGG2.0 are shown in Figure 26 for the three pesticides. The concentrations along the fracture (DF frac) as well as between two fractures (DF mid) are shown in red and purple respectively. The result for an EPM is shown in green.

With the simple model for transport through fractured media (JAGG2.0), it is possible to simulate the concentration profiles relatively well for the two monitoring rounds. Furthermore the presence of fractures can explain the detection of pesticides in the aquifer 25 meters below surface. With the EPM model, using the default parameters ( $\phi = 0.3$  and  $\alpha = 1\text{m}$ ), the maximum penetration in 2007 is around 15 mbs. However, as explained in the previous section, EPM model could also simulate the presence of pesticides in the groundwater using a smaller porosity and/or a larger dispersivity.

### 8.3 Chlorinated solvents source in fractured clay

Chlorinated solvents are a major threat to the groundwater resources in Denmark and many sites contaminated with chlorinated solvents occur in fractured clayey till overlying a secondary or primary aquifer. Several contaminated sites are used in this section to illustrate JAGG2.0.

#### 8.3.1 Sortebrovej - DNAPL source overlying a fractured clay till

The conceptual model 1a (Figure 8) is used to assess the contaminant flux from a contaminated clayey till to an upper sandy aquifer. The description of the site and the input data for the model are taken from Fynt Amt (2004). Free phase TCE was released in the 80's and the contaminant source is estimated to be located 4 m below ground surface and have an area of 80 m<sup>2</sup>. The total released residual mass is estimated to 20 kg TCE. The net infiltration in the area is estimated to be around 75 mm/year. In order to compensate for the uneven distribution of TCE in the source area, the solubility is assumed to be half of the theoretical solubility (700 mg/L). TCE is estimated to have leached from the free phase contaminant source for 5 years.

The average fracture spacing is estimated around 1 meter. By assuming that the porous matrix is impermeable, the corresponding fracture aperture has been calculated to be 30  $\mu\text{m}$ . The fracture velocity can be calculated from the net



infiltration ( $I$ ), the fracture spacing ( $2B$ ) and the fracture aperture ( $2b$ ):

$$v_f = I \frac{2B}{2b} = 2500 \text{ m/year} \quad (8.2)$$

The porosity of the clay matrix is estimated to be 30%, the tortuosity is assumed to be equal to the porosity. The free diffusion coefficient in water is  $6 \cdot 10^{-10} \text{ m}^2/\text{s}$  (US EPA 2009). The distribution coefficient  $K_d$  is estimated to be 0.062 L/kg, which corresponds to a retardation factor in the matrix of 1.4 (assuming a bulk density of 1.95 kg/L). A small amount of DCE was measured at the site and VC and ethene were detected in very limited amounts. Therefore TCE is assumed to degrade slowly to DCE, which is assumed to be non-degradable. The parameters used in JAGG2.0 are summarized in Table 10.

INPUT		
Input concentration	$C_0$ (mg/l)	700
Infiltration	$I$ (mm/year)	75
Fracture aperture	$2 \cdot b$ (m)	3.00E-05
Fracture spacing	$2 \cdot B$ (m)	1
Matrix porosity	$\phi$	0.3
Diffusion coefficient in matrix	$D_m$ ( $\text{m}^2/\text{year}$ )	0.00589
Degradation rate	$\lambda$ ( $\text{year}^{-1}$ )	0.01
Retardation, fracture	$R_f$	1
Retardation, matrix	$R_m$	1.4
Water velocity	$v_f$ (m/year)	2500
Spill time	$a$ (year)	5
Time	$t$ (year)	
Depth	$z$ (m)	16
Calculated parameters		
Bulk hydraulic conductivity	$K_b$ (m/s)	1.70E-08
Vertical gradient	$i$ (-)	0.14

Table 10 – Input parameters for Sortebrovej site

The concentration of TCE and DCE has been monitored between 1999 and 2005 in two boreholes located in the clayey till at 18 mbs, so JAGG2.0 is compared with these data for  $z = 14\text{m}$ , and the result is shown in Figure 27. It can be seen that the measured concentrations for TCE and DCE are between the simulated concentrations for the fracture and in the matrix at a distance of 0.5m from the fracture. Furthermore the results for the EPM model are very different with TCE concentration close to 0 and high concentration of DCE (above 30 mg/L). The EPM does not describe observed data, and so

the conceptual system of a fractured clayey till is valid for Sortebrovej site.

The vertical distribution of TCE in the clayey till is also compared with data measured in 2004 (around 25 years after the spill), and the result is shown in Figure 28. JAGG2.0 is in better agreement with the observation data than the EPM model although data scatter makes conclusion uncertain.

JAGG2.0 can be used for assessing the leaching concentration and duration from the clayey till into the upper sandy aquifer (Figure 29). However the risk posed to the regional aquifer, which is used for drinking water purposes cannot be directly assessed with JAGG2.0, as another clayey till layer is located between the sandy layer and the regional aquifer. The currently observed contamination corresponds to the modeled peak concentration of TCE, and AGG2.0 predicts that observed concentrations should now start decreasing slowly. In contrast JAGG2.0 predicts that the DCE concentration will keep increasing until a maximum of 3.5 mg/L around 2030. The concentration

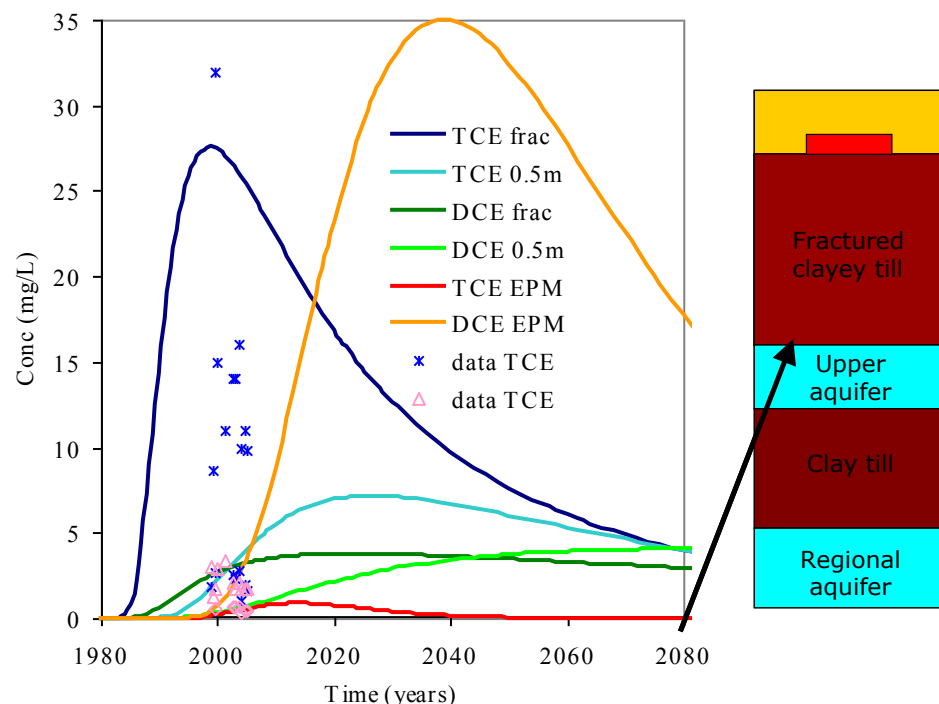


Figure 27 - TCE and DCE Concentrations in the clayey till at 18 mbs. TCE (and DCE) frac corresponds to the concentration at the fracture outlet (18 mbs), and TCE (and DCE) 0.5m corresponds to the concentration in the matrix (18mbs) at a distance of 0.5m from the fracture. Data from (Fyns Amt 2004).

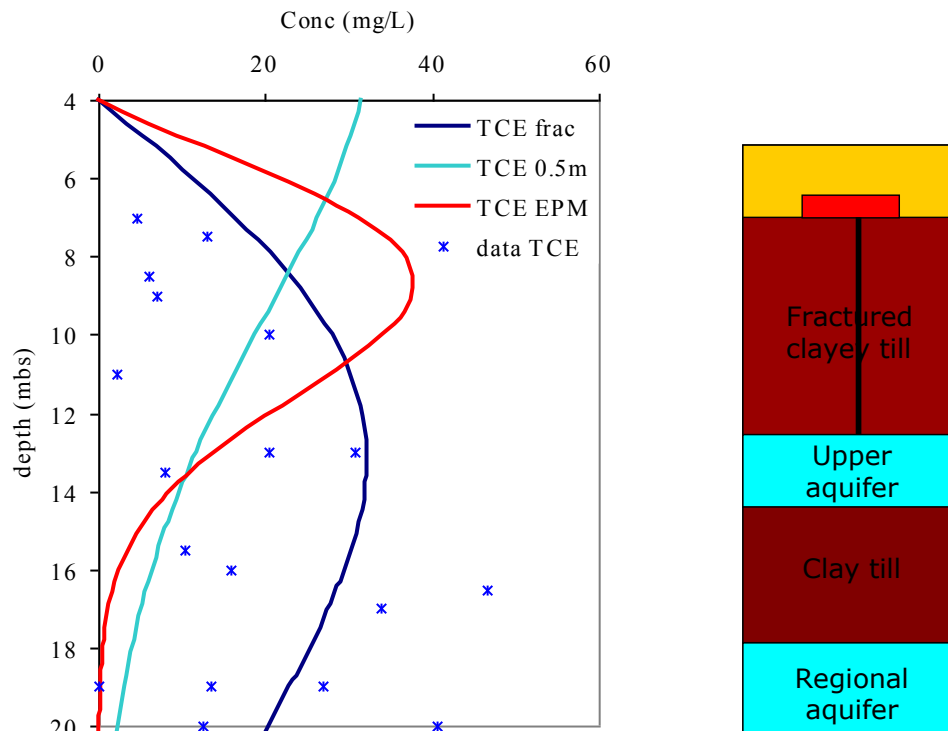


Figure 28 – Vertical TCE distribution 25 years after the spill.. TCE frac corresponds to the concentration along the fracture, and TCE 0.5m corresponds to the concentration in the matrix at a distance of 0.5m from the fracture. Data from (Fyns Amt 2004)

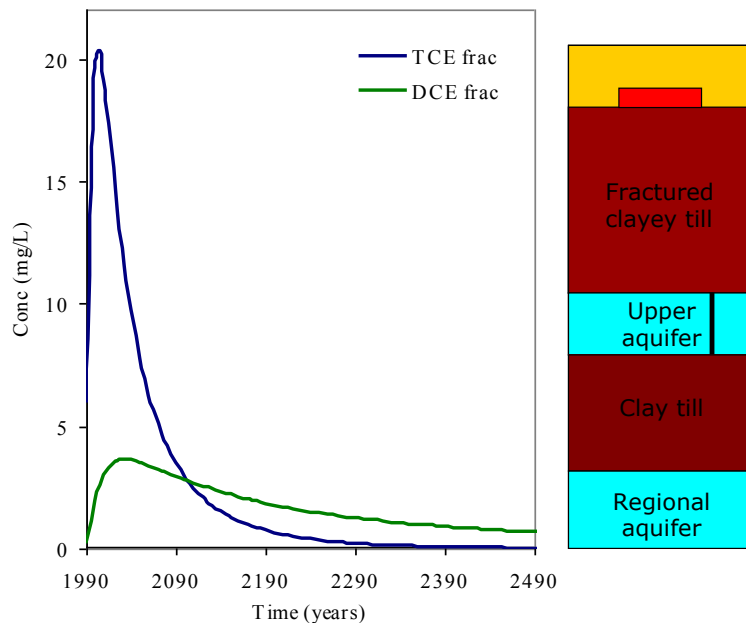


Figure 29 – Concentration leaching to the upper sandy aquifer

The resulting concentrations in the regional aquifer can be estimated, however the travel time from the upper aquifer to the regional aquifer is unknown. The dilution factor can be calculated with the equation:

$$DAF=1+\frac{K_{aq}i_{aq}d}{I \cdot L} \quad (8.3)$$

Where  $K_{aq}$  is the hydraulic conductivity of the aquifer,  $i_{aq}$  is the horizontal gradient,  $d$  is the mixing depth (or filter length to compare with measured data),  $I$  is the infiltration rate and  $L$  is the length of the source.

The hydraulic conductivity is taken at  $2.4 \times 10^{-4}$  m/s, the horizontal gradient at 3‰ (Fyns Amt 2004) and  $d$  is 3 m (filter length in the regional aquifer), which gives a dilution factor DAF of 100. The resulting concentrations in the regional aquifer are shown in Figure 30A. They are compared with measurement in the regional aquifer under the source area. The order of magnitude of the calculated concentration is comparable with the observations. The timing can be compared as the travel time from the upper to the regional aquifer is not taken into account in the calculations.

Assuming that all contaminant leaching from the source will reach the drinking wells located in the regional aquifer 200 meters from the contaminated site, and neglecting dispersion, the concentration in the wells can be estimated. The annual pumping rate is 130 000 m<sup>3</sup>/year (GEUS's Jupiter database). Again, the timeframe cannot be given as the travel time from the upper aquifer to the waterworks is unknown. It can however be seen that the total concentration at the waterworks is expected to be above 1 µg/L for a period of 10 years, before decreasing slowly over a period of 200 years to 0.1 µg/L.

JAGG2.0 shows that there is a risk of TCE and DCE contamination to the waterworks, if the contamination source is not remediated and if the water is flowing towards the drinking wells. However it has to be kept in mind that the available data for risk assessment are very limited and the parameter values are highly uncertain.

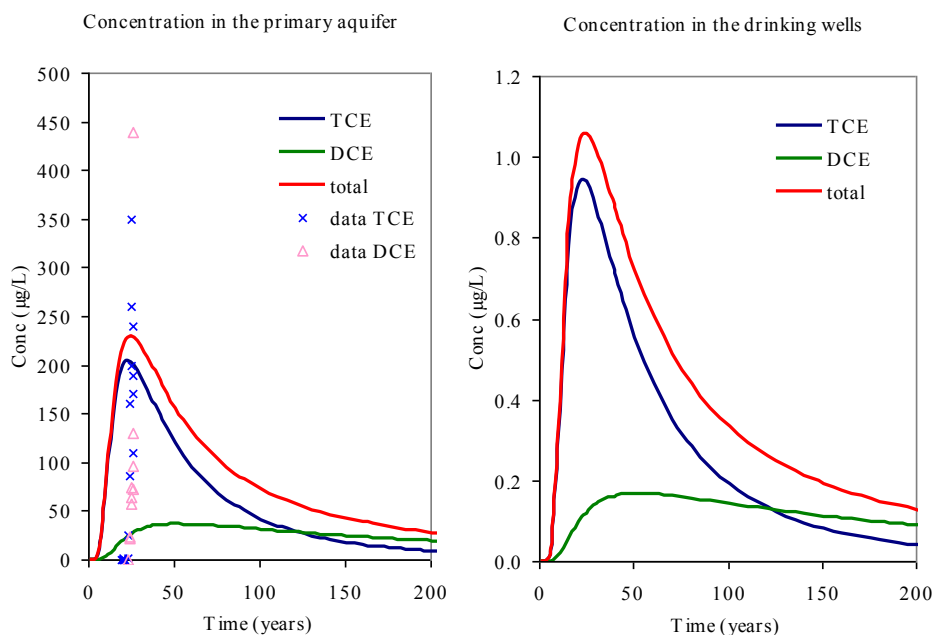


Figure 30 – A) Calculated concentration in the regional aquifer, and B) in the drinking wells, assuming that the whole leaching reaches the waterworks. Data from (Fyns Amt 2004)

Furthermore the results obtained with JAGG2.0 can be compared with results from numerical modeling made at the site by Manoli (2009). The expected peak concentration at the waterworks is comparable (around 1 µg/L), but the time of arrival and the extended duration of the peak due to dispersion (more than 60 years) cannot be predicted (see Figure 31).

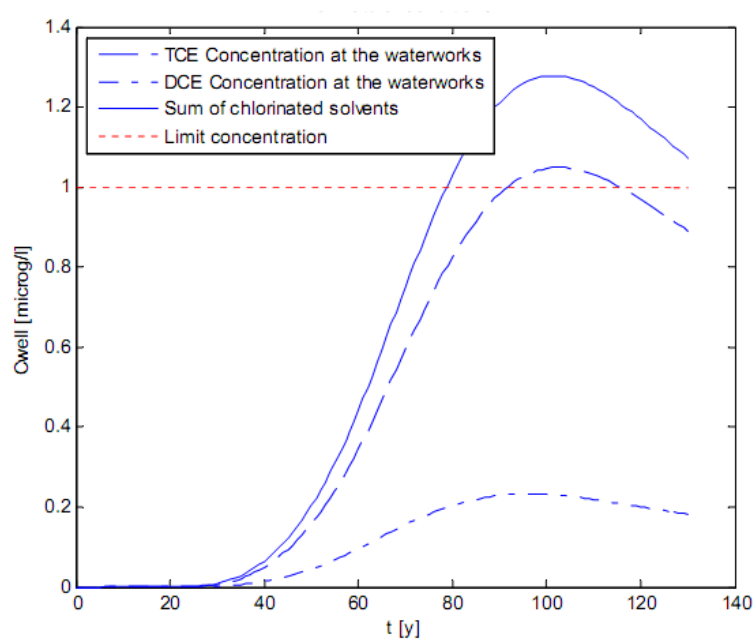


Figure 31 – Concentration at the waterworks simulated with numerical modeling using Comsol Multiphysics (Manoli 2009)

### 8.3.2 Gl. Kongevej - Contaminated clayey till with chlorinated solvents

At a former industrial site TCE has been used extensively and has led to the contamination of the saturated clayey till and to a lower extent of the underlying chalk aquifer (Miljøkontrollen 2004b). No physical source has been found at the site and the period during which TCE has spread is unknown, but the contaminant hotspot is located over an area of 140 m<sup>2</sup>, mainly in 5 meters of saturated clayey till which overlies the chalk regional aquifer. This corresponds to conceptual model 2 (see Figure 8). The main contaminant is TCE. The total mass of contaminant in the source zone is estimated to be 40 kg. Assuming a sorption coefficient  $K_d$  of 0.6 L/kg, a bulk density  $\rho_b$  of 1.96 kg/L and a porosity  $\phi$  of 0.3, the average aqueous concentration in the source zone is 40 mg/L. A vertical fracture spacing of 1 meter and aperture of 25  $\mu$ m are assumed, which together with the assumed recharge to the regional aquifer of 100 mm/year gives a velocity  $v_f$  of 4000 m/year.

#### Risk assessment

The conceptual model 2 is used to assess the leaching concentration to the regional aquifer, with the input parameters shown in Table 11.

INPUT		
Initial concentration	$CI$ (mg/l)	40
Infiltration	$I$ (mm/year)	100
Fracture aperture	$2*b$ (m)	2.50E-05
Fracture spacing	$2*B$ (m)	1
Matrix porosity	$f$	0.3
Diffusion coefficient in matrix	$D_m$ (m <sup>2</sup> /year)	0.00589
Degradation rate	$l$ (year <sup>-1</sup> )	0
Retardation, fracture	$R_f$	1
Retardation, matrix	$R_m$	4.92
Water velocity	$v_f$ (m/year)	4000
Time	$t$ (year)	
Depth	$z$ (m)	5
Calculated parameters		
Bulk hydraulic conductivity	$K_b$ (m/s)	9.83E-09
Vertical gradient	$i$ (-)	0.32

Table 11 – Input parameters for Gl. Kongevej

The concentration in the leachate decreases fast from 40 mg/L to 20 mg/L over a period of 20 years (see Figure 32), and has a long tailing with concentration above 10 mg/L for more than 150 years. In contrast, an EPM model predicts a constant concentration of 40 mg/L for a period of 50 years, followed by

a fast decrease to less than 1 mg/L after 100 years. The leachate concentration can be used to assess the concentration in the underlying chalk aquifer, assuming a hydraulic gradient of 3‰ and a hydraulic conductivity of  $5 \cdot 10^{-5}$  m/s for the aquifer (Miljøkontrollen 2004b). Assuming a mixing depth of 2m (length of monitoring well filter), the dilution factor calculated by Eq.(8.3) is equal to 8.9, which means that the groundwater quality criteria of 1µg/L will not be met in the chalk aquifer for the next 150 years (concentration will still be above 1 mg/L). However, as it has been noticed in Section 9.3, the leaching time is overestimated with the model, due to the assumption of single fracture and infinite storage in the adjacent matrix. The mass loading to the aquifer with JAGG2.0 is higher than predicted by EPM model due to the single fracture assumption, and the infinite contaminant storage in the matrix.

The results can also be compared with the observed TCE concentration in the regional aquifer in two monitoring boreholes (1.9 and 2.7 mg/L), and with the results from JAGG 1.5 (cf. Figure 33).

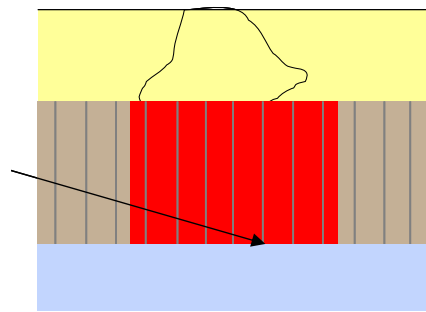
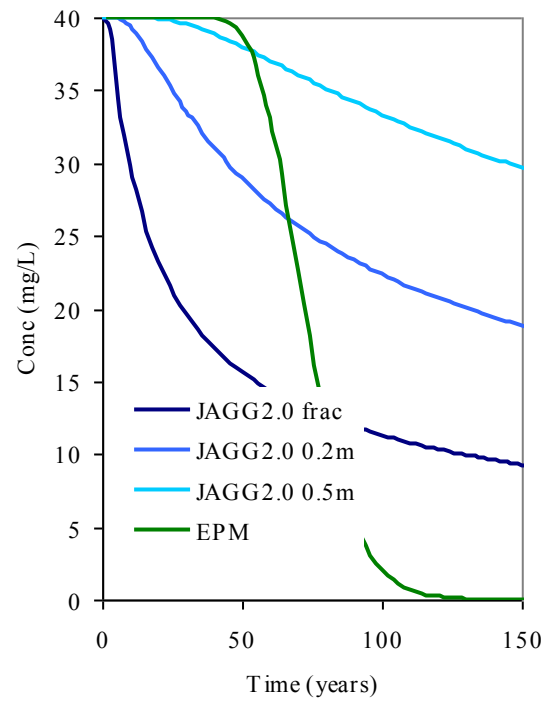


Figure 32 - TCE concentration at the fracture outlet and at 0.2 and 0.5 m from the fracture. The result from an EPM model is also shown (green).



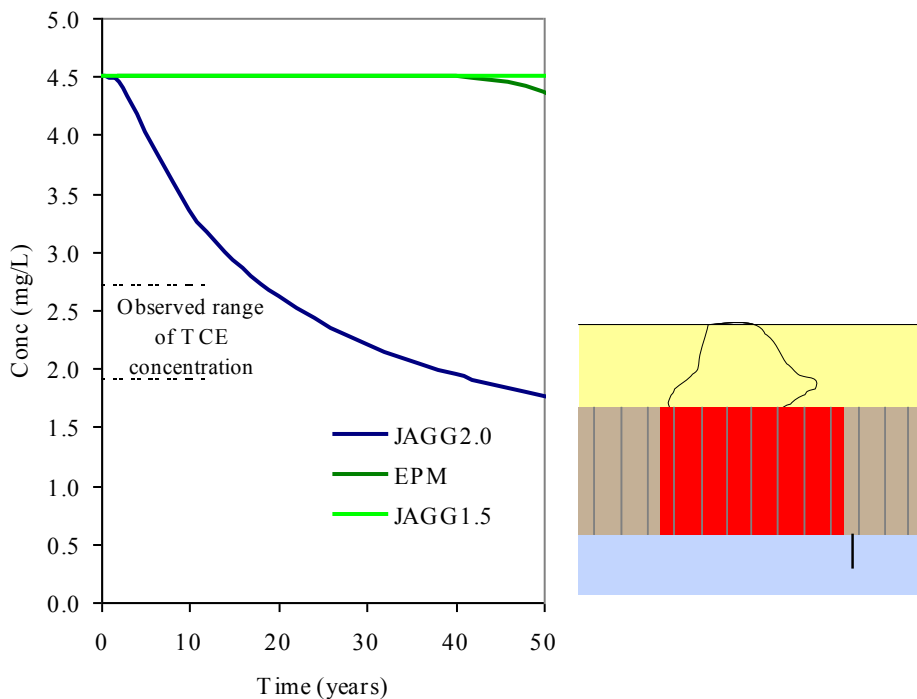


Figure 33 – TCE concentration in the regional aquifer (measured and predicted by JAGG2.0, JAGG 1.5 and EPM)

### Remediation

Anaerobic dechlorination was enhanced by the injection of molasses and specific degraders (including bacteria of the genus *Dehalococcoides*) in the contaminated zone in the clayey layer. JAGG2.0 can be used to assess the leaching concentration to the regional aquifer after enhancement of reductive dechlorination. However JAGG2.0 does not take into account the formation of daughter products (cis-DCE and VC) due to reductive dechlorination of TCE, and only TCE can be simulated. This can result in a poor assessment of remediation outcomes because the daughter products are more mobile than the parent compound TCE.

Several values for first-order degradation rates are used to simulate enhanced reductive dechlorination of TCE, and it can be seen that the leaching concentration is very sensitive to the value of degradation rate. From comparison with field data, it seems that dechlorination has been enhanced to a high degree in the contamination zone, with first-order rate between 5 and 10 yr<sup>-1</sup>, thus reducing the risk of TCE contamination in the aquifer and the source lifetime, compared to the zero degradation case. However JAGG2.0 does not take into account the formation of daughter products (cis-DCE and VC) due to reductive dechlorination of TCE.

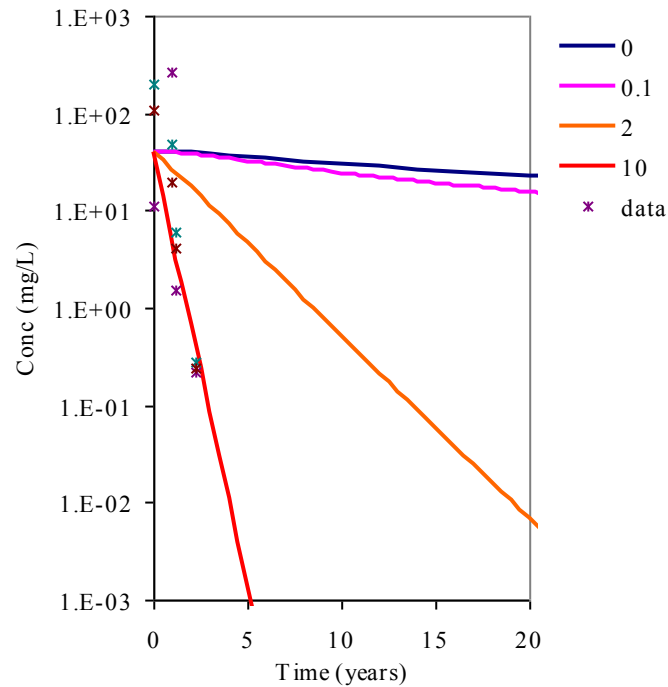


Figure 34 – Leaching concentration to the chalk aquifer for a variety of degradation rates, assuming that remediation starts at time 0. Measured concentrations at three boreholes in the source zone are also displayed. Note the log-scale of the vertical axis. Data from (Region Hovedstaden 2008)

It should be noted that for degradation rates above  $1.5 \text{ yr}^{-1}$ , the result of JAGG2 and the EPM model are equivalent to a simple exponential decay of the source concentration (see Figure 35) including no transport processes. This is due to the fact that the system is controlled by the degradation rate only.

The use of the conceptual model 2 for the case of degradation in the source zone is thus limited, as the result does not differ from a simple exponential decay model. Conceptual model 2 is mainly useful to assess the longevity of a source located in clayey till and the leaching concentration in case of a conservative or slowly degrading compound.

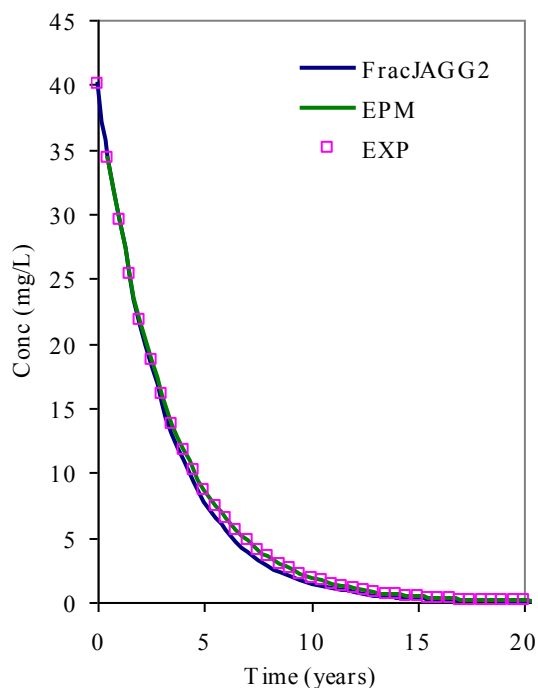


Figure 35 – Leaching concentration with degradation rate  $1.5 \text{ yr}^{-1}$ , for the fracture model, the EPM model and a simple exponential decay

#### 8.4 Contamination at gas stations (MTBE and benzene)

Risk assessment using JAGG1.5 has been performed at several gas stations for MTBE and benzene contamination in the aquifer in Miljøstyrelsen (2003). However at several sites, clayey till overlies the regional groundwater. The presence of fractures in this geological layer is not taken into account in the risk assessment performed using JAGG1.5. In this study, the JAGG2.0 is applied to such a site in order to illustrate the use of conceptual model 1b (Figure 8) and compare with results from JAGG1.5.

##### Ørkildsgade 52, 5700 Svendborg

MTBE and benzene have been measured in the source zone, which overlies a 15 meter thick clayey till. The input parameters for the two contaminants are taken from Miljøstyrelsen (2003) and summarized in Table 12.

INPUT		MTBE	Benzene				
Input concentration	$C_0$ (mg/l)	53	1.6	Conc (mg/L)			
Infiltration	$I$ (mm/year)	11	11	0.0	0.2	0.4	0.6
Fracture aperture	$2*b$ (m)	3.20E-05	3.20E-05	0			
Fracture spacing	$2*B$ (m)	2	2				
Matrix porosity	$\phi$	0.3	0.3	2			
Diffusion coefficient in matrix	$D_m$ (m <sup>2</sup> /year)	0.005317	0.00577109				
Degradation rate	$\lambda$ (year <sup>-1</sup> )	0	0.365	4			
Retardation, fracture	$R_m$	1	1				
Retardation, matrix	$R_f$	1.01625	1.0143	6			
Water velocity	$v_f$ (m/year)	688	688	8			
Time	t (year)						
Depth	z(m)	15	15	8			
Calculated parameters							
Bulk hydraulic conductivity	Kb (m/s)	1.03E-08	1.03E-08	10			
Vertical gradient	i (-)	0.03	0.03	12			

Table 12 – Input parameters for MTBE and Benzene in Svendborg

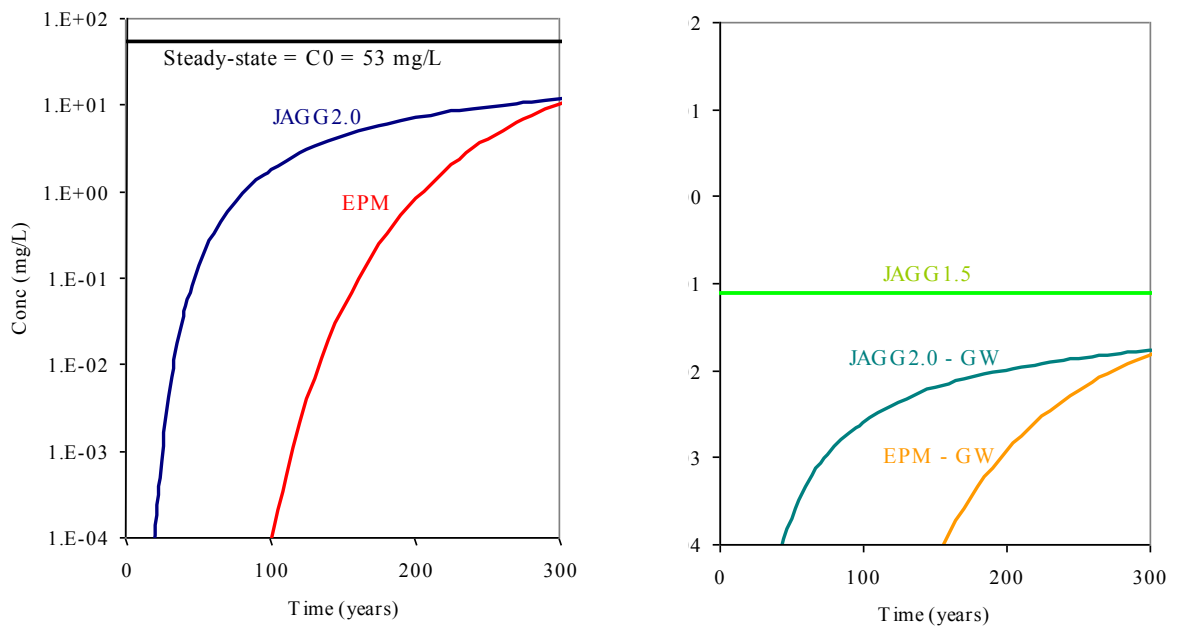


Figure 36 – MTBE concentration in water leaching from the fracture (left) and in the underlying regional aquifer (right), calculated by JAGG2.0 (transient in blue and steady-state in black), EPM (red and orange) and JAGG1.5 (green).

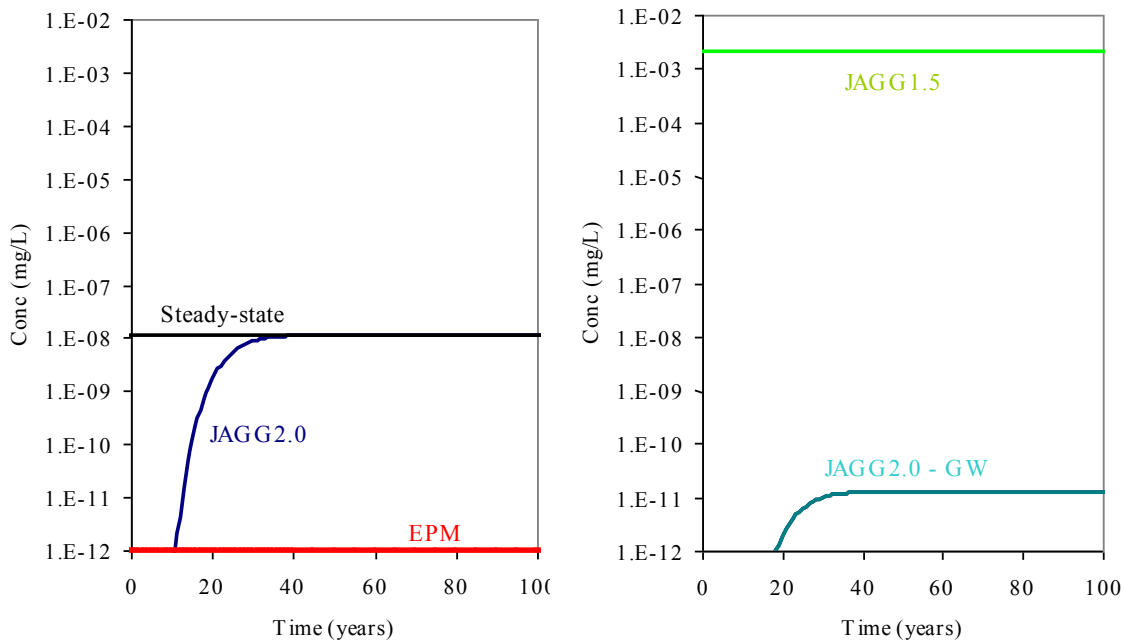


Figure 37 – Benzene concentration in water leaching from the fracture (left) and in the underlying regional aquifer (right), calculated by JAGG2.0 (transient in blue and steady-state in black), EPM (red) and JAGG1.5 (green).

For the conservative compound (MTBE in Figure 36), the results from JAGG2.0 are lower than from JAGG1.5 because the transient aspect is taken into account. It will take more than 300 years to reach the concentration predicted by JAGG1.5 in the groundwater.

Concerning the degradable compound (benzene in Figure 37), the results from JAGG2.0 are very different from JAGG1.5 as degradation during the vertical transport is not included in JAGG1.5. Therefore the risk in JAGG1.5 is overestimated and the results from the JAGG2.0 do not show benzene breakthrough in the aquifer (because of the degradation). Further discussion on the importance of the degradation processes can be found in Chapter 10.

## 9 Simplifications ( and consequences )

Transport in fractured media involves several complex processes, so that assumptions are necessary to simplify the mathematical problem and obtain the analytical solutions. In this chapter, these simplifications are discussed together with their consequences on the results in terms of risk assessment.

In all the examples presented in this chapter, the following parameters are used:

<b>Fracture aperture</b>	$2*b$ (m)	2.50E-05
<b>Fracture spacing</b>	$2*B$ (m)	1
<b>Matrix porosity</b>	$\phi$	0.3
<b>Diffusion coefficient in matrix</b>	$D_m$ (m <sup>2</sup> /year)	0.00589
<b>Degradation rate</b>	$\lambda$ (year <sup>-1</sup> )	0
<b>Retardation, fracture</b>	$R_f$	1
<b>Retardation, matrix</b>	$R_m$	1
<b>Aquifer hydraulic conductivity</b>	$K_{aq}$ (m/s)	1.00E-04
<b>Aquifer hydraulic gradient</b>	$iaq$	0.01
<b>Mixing depth</b>	$dm$ (m)	0.25

Table 13 – Parameters used in the following examples

### 9.1 Constant flow in the fracture

In JAGG2.0 the water flow in the fractured system is assumed to be at steady-state, with a constant water velocity along the fracture. With this assumption, the annual infiltration rate is employed and variations due to storm events are neglected. Storm events can result in a very high water velocity in the fracture and can greatly influence the risk assessment. This is illustrated for the two conceptual models (Figure 8) by simple examples, where different flow scenarios are considered:

- Scenario 1: Constant water flow with infiltration rate 120 mm/year
- Scenario 2: 2-days with 10 mm infiltration, followed by a constant infiltration of 110 mm for the rest of the year

JAGG2.0 cannot simulate variable flow. Scenario 2 (variable flow) is modeled with a numerical model in Comsol Multiphysics.

#### Conceptual model 1 (Figure 8)

A contamination source covering 1 m<sup>2</sup> (1\*1) is flushed at a constant concentration of 1mg/L. The source is overlying a 3 m thick fractured till. In these two scenarios, the annual infiltration rate (120 mm/year) and the inflow concentration (1mg/L) are the same, but the infiltration pattern is different with a non-constant water flow for scenario 2.

Scenario 1 (constant flow) and scenario 2 (variable flow) are compared for the case of the same contaminant load and the case of the same contamination duration. If the contaminant load is the same (20 mg), this means that for scenario 1 the source leaches for 2 months, while the source leaches for 2 days only for scenario 2. If the contamination duration is the same (2 days), this means that the contaminant load is 0.7 mg for scenario 1 and 20 mg for scenario 2.

The peak concentration in the underlying aquifer is higher for the storm event scenario than for the case of a constant water flow in the fracture (as shown in Figure 38). The assumption of a constant infiltration through the fractured clayey can thus lead to an underestimation of the concentration.

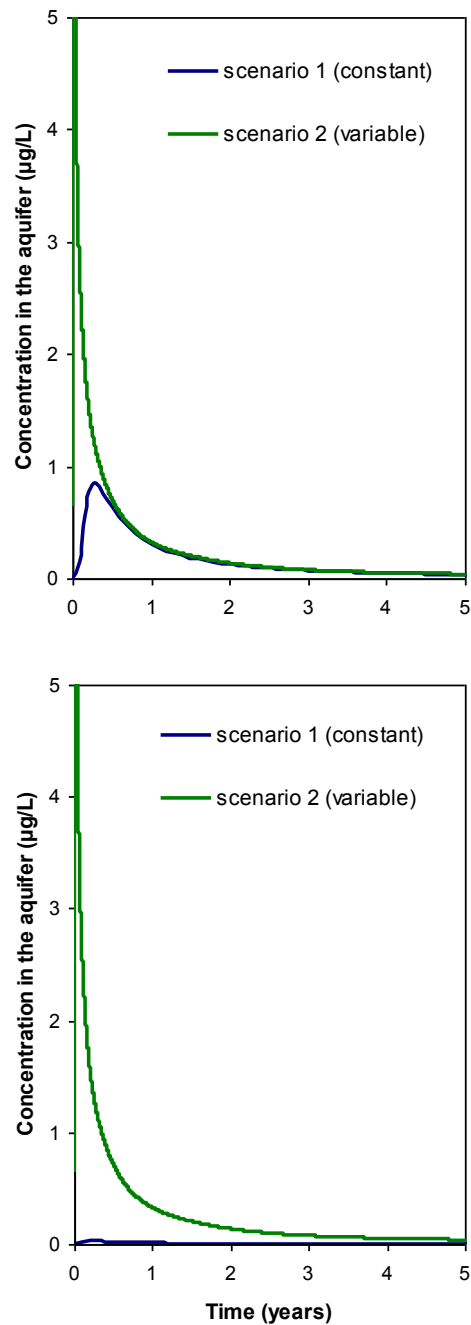


Figure 38 – Concentration in the underlying aquifer for the same load (left) or the same duration (right)

#### Conceptual model 2 (Figure 8)

A 5-meter thick fractured clay till is contaminated with a concentration of 1 mg/L. In this case, the concentration decreases slightly faster during scenario 2 due to a greater dilution in the water flowing along the fracture. The difference between constant and variable flow is small for this case.



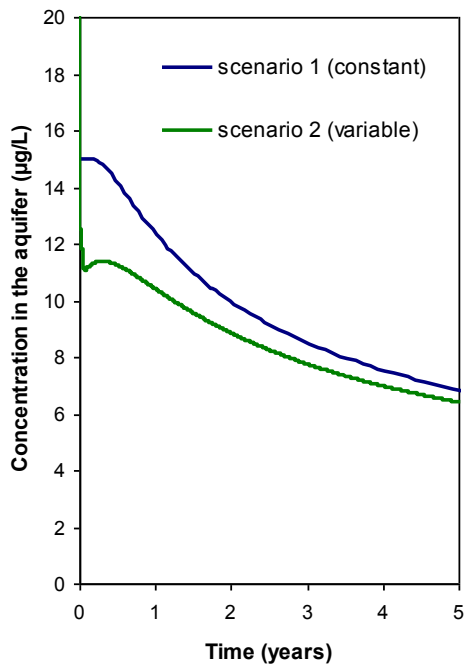


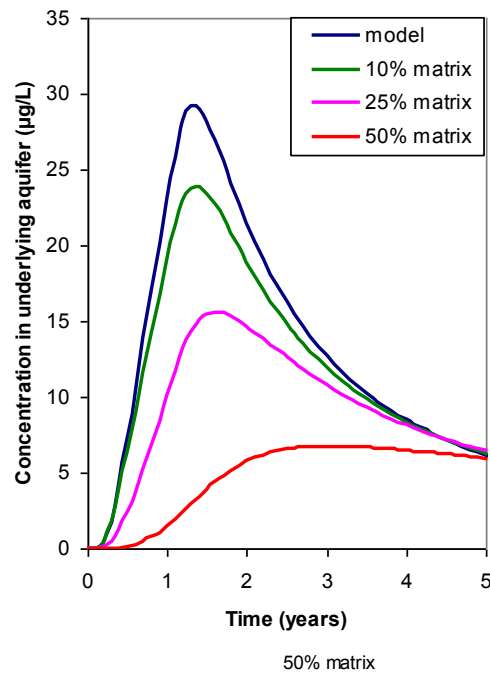
Figure 39 – Concentration in the underlying aquifer for constant and variable water flows for conceptual model 2

## 9.2 Negligible advection in the matrix

In JAGG2.0, the water flow is assumed to occur only along the vertical fractures and the matrix is impermeable. JAGG2.0 (where there is no water flow through the matrix) is compared with scenarios where water flows also through the matrix (10, 25 and 50% of the total infiltration rate) for conceptual models 1 and 2 shown in Figure 8. JAGG2.0 cannot simulate matrix flow. The scenarios with flow in the matrix are modeled with a numerical model in Comsol Multiphysics.

### Conceptual model 1 (Figure 8)

A contaminant source overlying a fractured till is leaching with a concentration of 1 mg/L for one year. JAGG2.0 overestimates the contaminant concentrations with fast contaminant breakthrough when advection in the matrix occurs (see Figure 40). Furthermore the advection in the matrix may create a second concentration peak when the contaminant mass in the matrix reaches the bottom of the fractured layer. This is illustrated in Figure 41 for the case where 50% of the water is flowing through the matrix.



( a 10 meter long source )

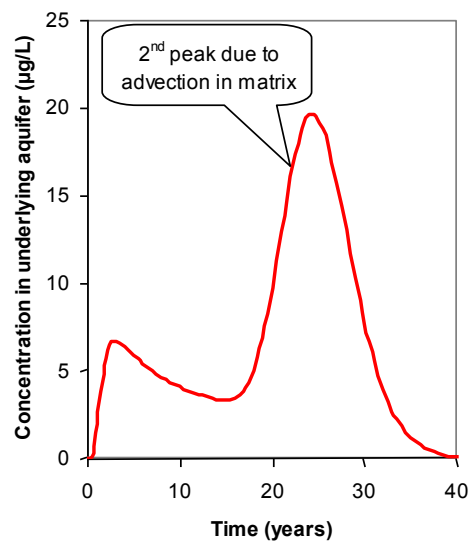


Figure 41 – Long-term concentration in the underlying aquifer when 50% of the water is flowing through the matrix by advection

### Conceptual model 2 (Figure 8)

A 5-meter deep fractured clay till is contaminated with a concentration of 1 mg/L. In this case the assumption of an impermeable matrix may underestimate the contaminant flux loading to the aquifer, as illustrated in Figure 42 below.

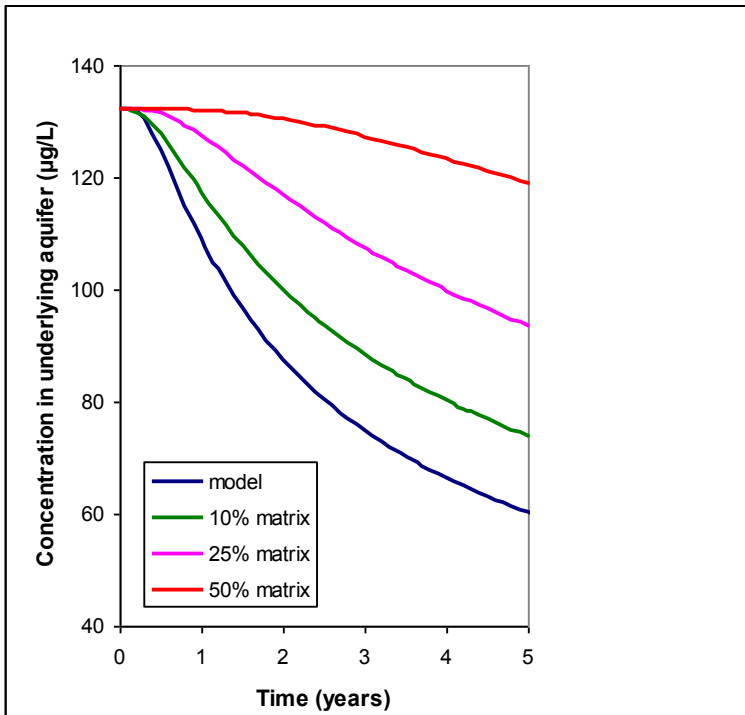


Figure 42 – Concentration in the underlying aquifer (assuming a 10 meter long source) for different water flows through the matrix

The percentage of water flowing through the matrix can be estimated by the ratio of the matrix hydraulic conductivity ( $K_m$ ) and the bulk hydraulic conductivity of the fractured media ( $K_b$ ). This check is implemented in JAGG2.0 where it is recommended that  $K_m/K_b < 10\%$ .

### 9.3 Single fracture vs. parallel fracture

In order to implement the fracture module JAGG2.0 in Excel, it was necessary to simplify the governing equations by assuming a single fracture surrounded by an infinite porous matrix. The simplification results in an underestimation of the concentration in the fracture for models 1a and 1b, because the storage capacity of the matrix is finite and the attenuation due to diffusion into the matrix is higher with an infinite fracture spacing than for the case of parallel fractures. However for large fracture spacing ( $2B$ ) the maximum penetration depth of the contaminant inside the matrix (corresponding to steady-state) is less than  $B$ , and the two systems are equivalent. This can be seen by comparing the steady-state concentration for model 1b in the fracture for a single fracture system calculated using Eq.(9.2) and a for parallel fracture system where the concentration is (Sudicky and Frind 1982):

$$\frac{C_{f-//}}{C_0} = \exp\left(-\frac{\lambda z}{v_f}\right) \exp\left(-\frac{H\sqrt{\lambda/R_m}}{A} \tanh\left(\sqrt{\lambda/D_m}(B-b)\right)\right) \quad (9.1)$$

$$\frac{C_{f-single}}{C_0} = \exp\left(-\frac{\lambda z}{v_f}\right) \exp\left(-\frac{H\sqrt{\lambda/R_m}}{A}\right) \quad (9.2)$$

This can be shown by noting that:

$$\begin{aligned} C_{f-//} \rightarrow C_{f-single} &\Leftrightarrow \tanh\left(\sqrt{\lambda/D_m}(B-b)\right) \rightarrow 1 \\ &\approx \tanh\left(\sqrt{\lambda/D_m}(B-b)\right) > 0.95 \\ &\approx \sqrt{\lambda/D_m} B > 1.83 \quad (B \gg b) \end{aligned} \quad (9.3)$$

The solution for a system of parallel fractures tends to the solution for a single fracture when  $\tanh\left(\sqrt{\lambda/D_m}(B-b)\right)$  tends to

1. Assuming an error of 5%, this is equivalent to

$\tanh\left(\sqrt{\lambda/D_m}(B-b)\right)$  equal 0.95. Furthermore in most of systems, B is much larger than b (the spacing is much larger than the fracture aperture), so that  $\tanh\left(\sqrt{\lambda/D_m}(B-b)\right)$  can be approximated by  $\tanh\left(\sqrt{\lambda/D_m} B\right)$ .

The parallel fracture system will become equivalent to the single fracture system for increasing spacing ( $2B$ ) and first-order degradation rate ( $\lambda$ ).

This is illustrated for the example shown in Figure 43 with the following parameters:

$$\begin{aligned} D_d &= 10^{-10} \text{ m}^2/\text{s} & \phi &= 0.3 \\ R_f &= 1 & R_m &= 5 \\ 2b &= 100 \text{ } \mu\text{m} & v_f &= 1 \text{ m/d} \\ z &= 5 \text{ m} \end{aligned}$$

For a conservative compound, the single fracture model is equivalent to the parallel fractures system for spacing larger than 0.8 meters, whereas this value decreases to 0.4 meters for a slow degradable compound ( $\lambda = 0.1 \text{ yr}^{-1}$ ). The minimum fracture spacing required for equivalence decreases fast with increasing degradation rates.

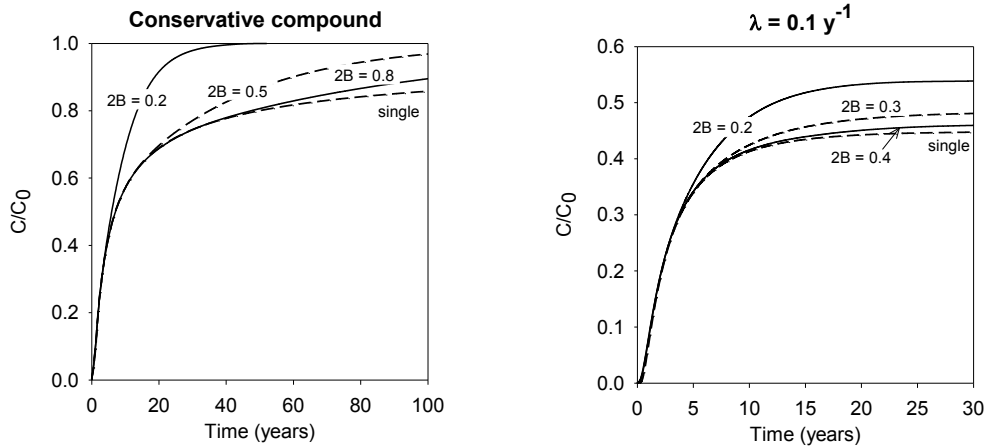


Figure 43 – Breakthrough curves of model 1b at  $z = 5$  m for a conservative ( $\lambda = 0$ ) and a degradable compound ( $\lambda = 0.1 \text{ yr}^{-1}$ ), and various fracture spacings. Note different time scales.

For conceptual model 2 an overestimation of the leaching time will be observed, as the matrix is infinite in the horizontal direction. This is illustrated in Figure 44, which compares the leaching concentration from JAGG2.0 (single fracture) with the numerical solution for a fracture spacing of 1 m (using the parameters from Table 13). The concentration in the fracture is well simulated for 20 years, but large difference between single and parallel fractures appears at time above 25 years.

Furthermore, the concentration at a distance of 0.5 meter from the fracture calculated by the two models is very different, with on overestimation of concentration being more significant with increasing time in case of a single fracture. The assumption of a single fracture embedded in a semi-infinite matrix results in an overestimation of the contaminant mass loading to the aquifer (grey zone in Figure 44). The mass leaching from the fractured media can then be higher than the initial mass in the system.

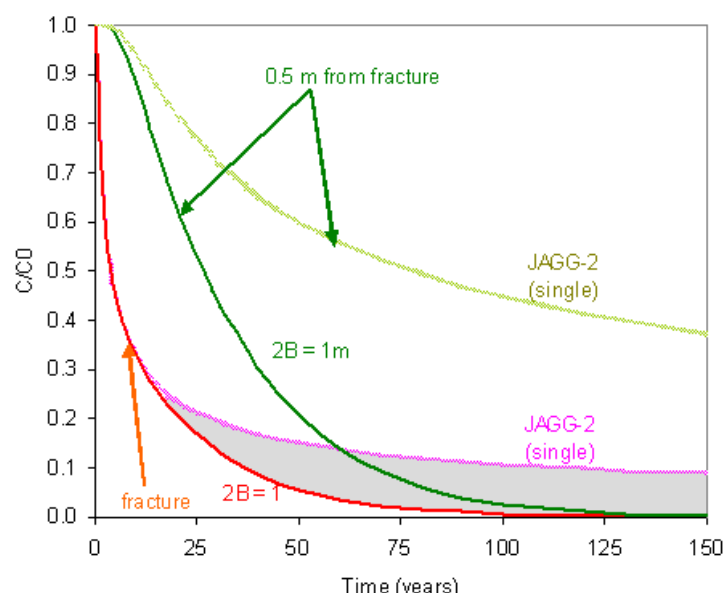


Figure 44 – Breakthrough curve for model 2 (uniform initial concentration in fractured media) for JAGG2.0 and for a spacing of 1m. The grey zone indicates the overestimation of mass loading to the aquifer.

In low-permeability deposits such as glacial tills, the vertical fracture spacing increases fast with increasing depth, and is expected to be above 1 meter at 5 meters below surface (Ruland et al. 1991, Jørgensen et al. 2003). This means that the results for model 1 are similar for most cases to the parallel fractures solution. Although the results for model 2 are overestimated, it gives useful information of the concentration and the leaching time. Therefore the single fracture model is a reasonable approximation for a risk assessment study.

#### 9.4 Uniform degradation in fracture and matrix

In JAGG2.0, the first order degradation rate is assumed to be constant and uniform in the fracture and matrix. However, the degradation is often microbially-driven and hence depends on the presence of microorganisms in the system. Research is currently conducted to determine the ability of the microbe to migrate and grow in low-permeability deposits, such as clay matrix. The use of uniform biodegradation of contaminant in the matrix is a simplification, which has not been verified. Intact core samples taken in clayey till tend to show that biodegradation is localized in bioactive zones close to the fractures and sand lenses (Region Syddanmark 2007, Region Syddannemark 2008). Furthermore it has been shown in Miljøstyrelsen (2009a) that the localization of the biodegradation in the clay matrix greatly influences the concentration leaching to the underlying aquifer, as well as the contamination length.

The assumption of a uniform degradation rate in the fracture and matrix can therefore lead to an overestimation of the contaminant attenuation and an underestimation of the risk posed to the groundwater.

#### 9.5 Overview of results

<b>Simplification</b>	<b>Model</b>	<b>Effects</b>
Constant water flow	1	Lower concentration Shorter leaching time
	2	Small effect (slightly) higher concentration
Negligible advection in matrix	1	Higher concentration Shorter leaching time
	2	Lower concentration Shorter leaching time
Single fracture	1	Small effect for $2B > 1m$ Lower concentration
	2	Infinite leaching time Higher mass loading to aquifer
Uniform degradation	1&2	Lower concentration Longer leaching time

Table 14 – Overview of results in chapter 9

# 10 Importance of degradation processes

One of the main novelties in JAGG2.0 is the inclusion of degradation processes during the vertical transport to the aquifer. Degradation processes are also included in the developed module for fractured media, and the importance of these processes in term of risk assessment is discussed in this chapter. As explained in Section 9.4, the degradation is assumed to be uniform in the fractured media (fracture and matrix). Conceptual model 1a (Figure 8) is used to illustrate the importance of degradation processes in the fracture module of JAGG2.0. The parameters used in this chapter are shown in Table 15.

INPUT		
Input concentration	$C_0$ (mg/l)	1
Infiltration	$I$ (mm/year)	35
Fracture aperture	$2*b$ (m)	2.50E-05
Fracture spacing	$2*B$ (m)	1
Matrix porosity	$\phi$	0.3
Diffusion coefficient in matrix	$D_m$ (m <sup>2</sup> /year)	0.006
Degradation rate	$\lambda$ (year <sup>-1</sup> )	
Retardation, fracture	$R_f$	1
Retardation, matrix	$R_m$	2
Water velocity	$v_f$ (m/year)	1400
Spill time	$a$ (year)	10
Time	$t$ (year)	
Depth	$z$ (m)	5

Table 15 – Input parameters used in Chapter 10

The degradation during transport through fractured media is an important process, both in term of peak concentration and leaching time. The concentration in the fracture outlet (at 5 meters depth) is shown in Figure 45 for different degradation rates. The peak concentration is divided by 100 between a non-degradable compound and a compound degrading with a rate of 1 year<sup>-1</sup>. The leaching time is also reduced with degradation. This is due to the fact the compound penetrates less in the matrix due to degradation, as illustrated in Figure 46, which shows the concentration in the matrix at a distance of 0.5m from the fracture.



The degradation rates can be much higher for some compounds, as for ex. benzene ( $\lambda = 3.6 \text{ yr}^{-1}$ ) (Miljøstyrelsen 2007), resulting in significant concentration attenuation at the bottom of the fractured media.

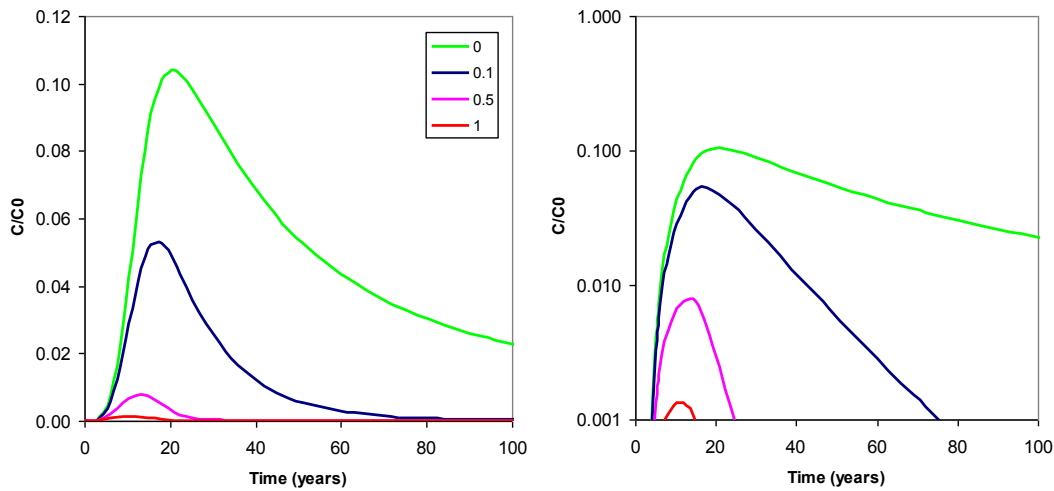


Figure 45 – Concentration in the fracture outlet (at 5 meters depth) as a function of the degradation rate (in 1/year). Note the log y-axis for the graph on the right

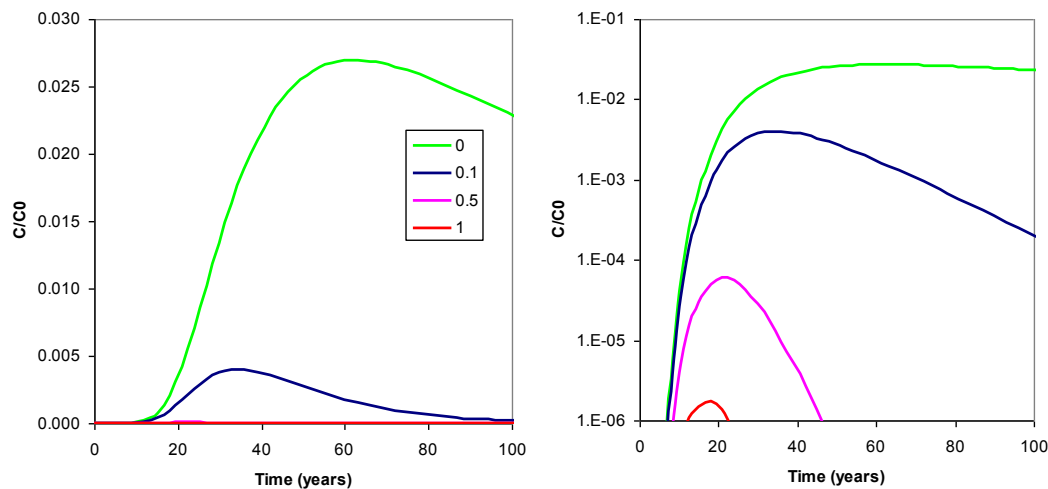


Figure 46 – Concentration in the matrix at a distance of 0.5m from the fracture (at 5 meters depth) as a function of the degradation rate (in 1/year). Note the log Y-axis for the graph on the right

The examples above show that degradation processes have a significant impact on risk assessment. However this is the case under the assumption of uniform degradation in the fracture and matrix. It was shown in Chambon et al. (2010), that attenuation is negligible if degradation occurs in the fractures only.

# 11 Is the risk assessment conservative?

Due to the many uncertainties related to risk assessments, approaches that ensure that conservative but realistic results are obtained, are preferable. In the present case, the developed specific tool for fractured media should be compared with the generally used equivalent porous media (EPM) model. As discussed in the previous chapters, it is not possible to conclusively validate the developed model for fractured media (vs. EPM) based on the available data. An important consideration in risk assessment in fractured media should be to ensure that any uncertainty is expressed as an over- and not under-estimation of the risk. However the notion of risk can be difficult to define objectively and depends on interpretations and situations. For example, is it more risky to have high concentration for a short period or low concentration for a long period (as illustrated in Figure 47 below)? Furthermore in case of a transient concentration (as the results from JAGG2.0), the notion of risk depends also on the time at which it is considered.

Conclusions on these considerations are beyond the scope of this project; therefore EPM and JAGG2.0 are compared in this chapter only in terms of peak concentration and leaching time.

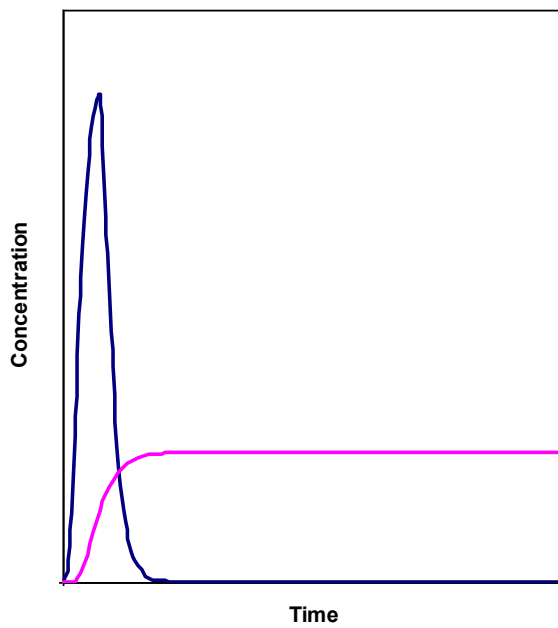


Figure 47 –concentration in the fracture outlet entering the aquifer under different conditions. This illustrates two different notions of risk: high concentration for a short period (blue) or lower concentration for a long period (pink), which one is the more risky?

The parameters used in this chapter are shown in Table 16.

<b>INPUT</b>		
<b>Input concentration</b>	$C_0$ (mg/l)	1
<b>Infiltration</b>	$I$ (mm/year)	35
<b>Fracture aperture</b>	$2*b$ (m)	2.50E-05
<b>Fracture spacing</b>	$2*B$ (m)	1
<b>Matrix porosity</b>	$\phi$	0.3
<b>Diffusion coefficient in matrix</b>	$D_m$ (m <sup>2</sup> /year)	0.006
<b>Degradation rate</b>	$\lambda$ (year <sup>-1</sup> )	0
<b>Retardation, fracture</b>	$R_f$	1
<b>Retardation, matrix</b>	$R_m$	2
<b>Water velocity</b>	$v_f$ (m/year)	1400
<b>Time</b>	$t$ (year)	
<b>Depth</b>	$z$ (m)	5

Table 16 – Input parameters used in Chapter 11

### 11.1 Non-degradable compounds

The breakthrough curves at 5 meters depth for a non-degradable compound for the three conceptual models are shown in Figure 48.

For conceptual model 1 (source overlying fractured media, Figure 8), the EPM model predicts a higher peak concentration. The breakthrough curves from JAGG2.0 are attenuated due to diffusion into the porous matrix. Also, JAGG2.0 predicts an earlier breakthrough to the underlying aquifer (20 vs. 70 years for model 1a).

For conceptual model 2, JAGG2.0 predicts a faster concentration decrease than the EPM model. On the other hand the contaminant leaching is expected to last longer in case of a fracture model (>300 vs. 200 years). The mass loading to the aquifer for conceptual model 2 is higher with JAGG2.0 than with an EPM model, due to the assumption of a single fracture (see Section 9.3).

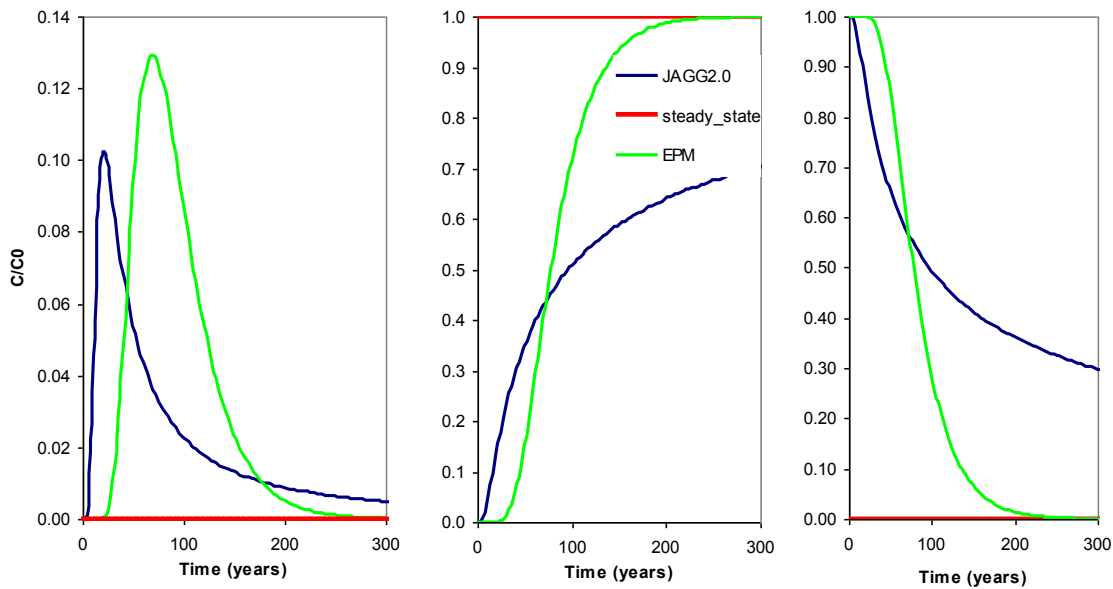


Figure 48 – EPM vs. JAGG2.0 for the three conceptual models (1a, 1b and 2) for a conservative compound. The concentrations in the fracture outlet (at 5 meters depth) calculated by JAGG2.0 is shown in blue, while the steady-state and EPM are shown in red and green.

## 11.2 Degradable compounds

The breakthrough curves at 5 meters depth for a slowly degradable compound ( $\lambda = 0.1 \text{ yr}^{-1}$ ) for the three conceptual models are shown in Figure 49. In case of a degradable compounds (even with a very slow degradation rate), the EPM model predicts a very high attenuation and the peak concentration is 5 times lower than for JAGG2.0. If the degradation rate is increased (to  $\lambda = 1 \text{ yr}^{-1}$  for example), the EPM model does not predict contaminant breakthrough at the bottom of the 5 meters clay till (Figure 50).

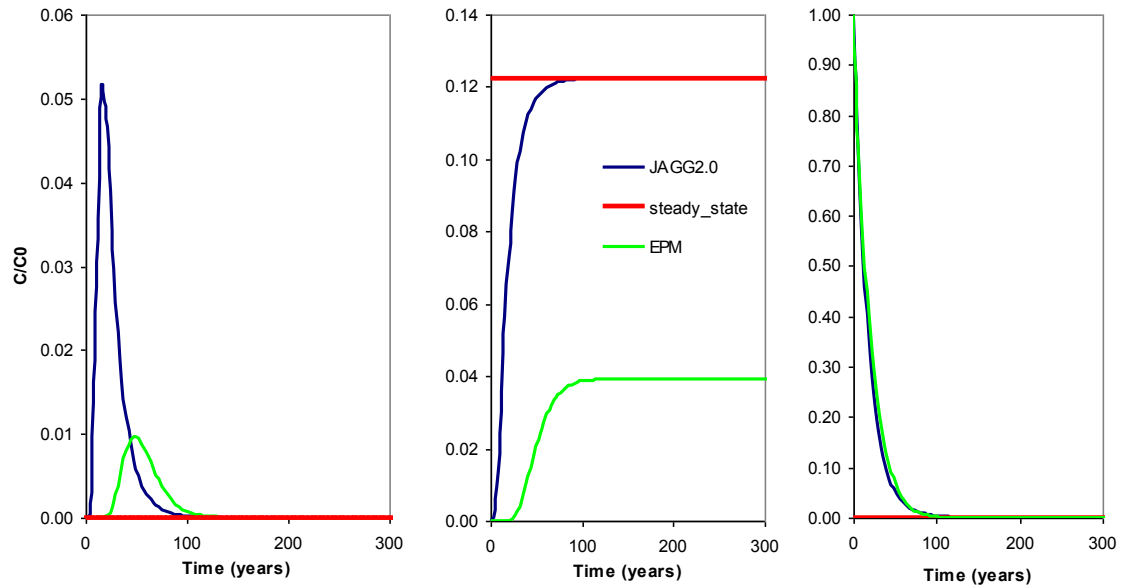


Figure 49 – EPM vs. JAGG2.0 for the three conceptual models (1a, 1b and 2) for a slowly degradable compound ( $\lambda = 0.1 \text{ yr}^{-1}$ )

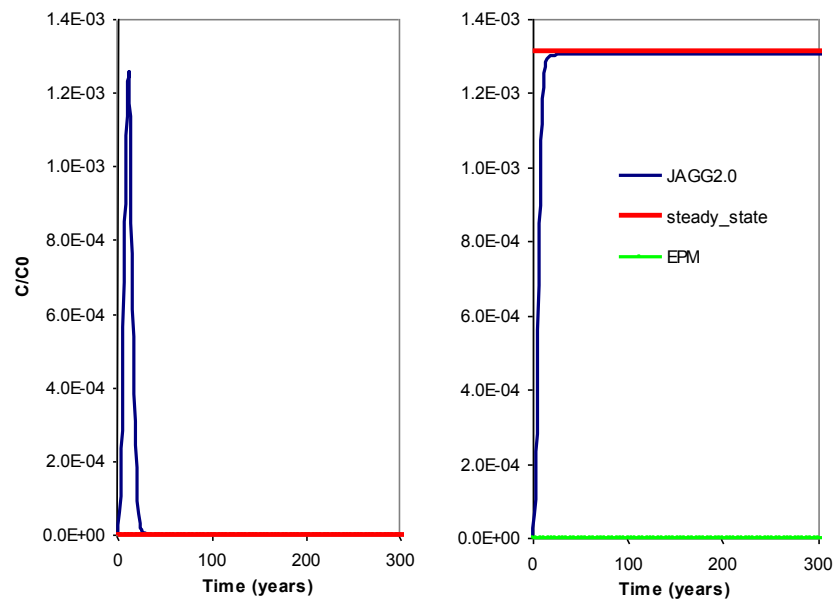


Figure 50 – EPM vs. JAGG2.0 for conceptual model 1(1a and 1b) for a degradable compound ( $\lambda = 1 \text{ yr}^{-1}$ )

### 11.3 Implication for risk assessment

The behavior of the two approaches (JAGG2.0 and EPM) is very different for non-degradable and degradable compounds. For non-degradable compounds, the EPM model will tend to provide the most conservative results, compared to JAGG2.0 for conceptual model 1a and 1b. The peak concentration from JAGG2.0 are around 20-30 % lower than the results from EPM model. For conceptual model 2, higher concentrations are achieved by the EPM model, however, the leaching will

continue much longer according to Figure 46. What is then the most conservative prediction?

In contrast, the use of EPM model in case of degradable compounds will result in an underestimation of the risk posed to the underlying aquifer. In this case, the results from JAGG2.0 are the most conservative.

In conclusion, none of the models considered in this report is always conservative. The use of the simple models presented in this report for risk assessment purposes should therefore always be done with care.

For practical purposes the following recommendations can be made for performing risk assessment with JAGG 2.0.

- Case 1: a source can be identified on site and concentration data in this source are available. It is then recommended to use model 1b for risk assessment and to use the maximum measured concentration in the source as input concentration ( $C_0$ ) in the underlying fractured media.
- Case 2: the physical source cannot be found and only concentrations in the fractured media can be measured (see example on Gl. Kongevej, Section 8.3.2). It is then recommended to use model 2 for risk assessment and to use the maximum concentration in the fractured media as homogeneous initial concentration ( $C_i$ ).

The inclusion of degradation in the risk assessment process has to be done with caution, as little is known on degradation in fractured media, and recent studies have shown that degradation may not occur homogeneously in the matrix (Chambon et al. 2010).

Model 1a is not suitable for risk assessment but can be applied to assess the effect of remedial action, in particular source removal, on the risk posed to the aquifer.

# Reference list

Chambon, J., Broholm, M.M., Binning, P.J., and Bjerg, P.L., 2010, *Modeling multi-component transport and enhanced anaerobic dechlorination processes in a single fracture - clay matrix system*, Journal of Contaminant Hydrology 112, 77-90.

Chen, C.T. and Li, S.H., 1997, *Radionuclide transport in fractured porous media - Analytical solutions for a system of parallel fractures with a constant inlet flux*, Waste Management 17[1], 53-64.

Fyns Amt, 2004, *Undersøgelser til vurdering af stimuleret in-situ reduktiv deklorering og kemisk oxidation ved oprensning af grundvandsforurening - Forurenet lokalitet nr. 485-20 Tidligere maskinfabrik Sortebrovej 26, 5690 Tommerup*, Hedeselskabet.

Harrar, W.G., Murdoch, L.C., Nilsson, B., and Klint, K.E.S., 2007, *Field characterization of vertical bromide transport in a fractured glacial till*, Hydrogeology Journal 15[8], 1473-1488.

Hinsby, K., McKay, L.D., Jørgensen, P., Lenczewski, M., and Gerba, C.P., 1996, *Fracture aperture measurements and migration of solutes, viruses, and immiscible creosote in a column of clay-rich till*, Ground Water 34[6], 1065-1075.

Jørgensen, P.R., McKay, L.D., and Spliid, N.H., 1998, *Evaluation of chloride and pesticide transport in a fractured clayey till using large undisturbed columns and numerical modeling*, Water Resources Research 34[4], 539-553.

Jørgensen, P.R., Hoffmann, M., Kistrup, J.P., Bryde, C., Bossi, R., and Villholth, K.G., 2002, *Preferential flow and pesticide transport in a clay-rich till: Field, laboratory, and modeling analysis*, Water Resources Research 38[11].

Jørgensen, P.R., Klint, K.E.S., and Kistrup, J.P., 2003, *Monitoring well interception with fractures in clayey till*, Ground Water 41[6], 772-779.



Manoli, G., 2009, Modelling the timeframe for remediation of a contaminated site located in a clay till, MSc Thesis, DTU Environment..

Mckay, L.D., Cherry, J.A., and Gillham, R.W., 1993, *Field Experiments in A Fractured Clay Till .1. Hydraulic Conductivity and Fracture Aperture*, Water Resources Research 29[4], 1149-1162.

Mckay, L.D., Stafford, P.L., and Toran, L.E., 1997, *EPM modeling of a field-scale tritium tracer experiment in fractured, weathered shale*, Ground Water 35[6], 997-1007.

Miljøkontrollen, 2000, *Point and non-point source leaching of pesticides in a till groundwater catchment*, Vejledning fra Miljøstyrelsen, Danish Pesticide Research Programme.

Miljøkontrollen, 2004a, *Gammel Kongevej 39, Indledende forureningsundersøgelse*, Hedeselskabet.

Miljøkontrollen, 2004b, *Gammel Kongevej 39, Supplerende forureningsundersøgelse*, Hedeselskabet.

Miljøstyrelsen, 1998, *Oprydning på lokaliteter - Hovedbind*, Report Nr. 6, Vejledning fra Miljøstyrelsen.

Miljøstyrelsen, 2002a, *Kilder til BAM-forurening og forureningsudbredelse. Undersøgelseserfaringer. Delrapport 2*, Report Nr. 34, HOH Vand og Miljø A/S.

Miljøstyrelsen, 2002b, *Pesticider og vandværker. Udredningsprojekt om BAM-forurening. Hovedrapport*, Report Nr. 732, HOH Vand og Miljø A/S, GEO, DTU Miljø, København Universitet, Geologisk Institut, and Danmarks Jordbrugsforskning.

Miljøstyrelsen, 2002c, *Vurdering af koncentration og varighed af BAM-forurening i Grundvand. Delrapport 4*, Report Nr. 36, København Universitet, Geologisk Institut.

Miljøstyrelsen, 2003, *Risikovurdering af MTBE-forurening i forhold til grundvandet. Hovedrapport*, Report Nr. 785, Teknologiuudviklingsprogrammet for jord- og grundvandsforurening., Rambøll A/S.

Miljøstyrelsen, 2007, *Opgradering af JAGG til version 2.0 - Vertikal transport ned til førstkomende betydende magasin*, Teknologiudviklingsprogrammet for Jord- og Grundvandsforurening, Niras A/S. (Udkast).

Miljøstyrelsen, 2009a, *Model assessment of reductive dechlorination as a remediation technology for contaminant sources in fractured clay: Modeling tool. Delrapport II*, Teknologiprogram for jord- og grundvandsforurening, DTU Miljø.

Miljøstyrelsen, 2009b, *En pesticidforurening 15 år efter - spredning, nedbrydning og akkumulation i jordsølen*, GEO and Aarhus Universitet.

Mortensen, A.P., Jensen, K.H., Nilsson, B., and Juhler, R.K., 2004, *Multiple tracing experiments in unsaturated fractured clayey till*, Vadose Zone Journal 3[2], 634-644.

Region Hovedstaden, 2008, *Gl Kongevej 39 Status for monitorering af afværge*, Orbicon A/S, Roskilde.

Region Syddanmark, 2007, *Oprensning af klorerede opløsningsmidler i moræneler med stimuleret reduktiv deklorerung - Pilotforsøg - Rugårdsvej 234-238, Odense*, Cowi, DTU and Geosyntec.

Region Syddannemark, 2008, *Videregående monitorering af oprensning på Sortebrovej - Kerneprøvetagning 2008*, Notat, DTU Miljø.

Ruland, W.W., Cherry, J.A., and Feenstra, S., 1991, *The Depth of Fractures and Active Groundwater-Flow in A Clayey Till Plain in Southwestern Ontario*, Ground Water 29[3], 405-417.

Schmelling, S.G. and Ross, R.R., 1996, *Contaminant Transport in Fractured Media: Models for Decision Makers*, EPA Environmental assessment sourcebook, [10], 163-173. CRC Press.

Shih, D.C.F., Lin, G.F., and Wang, I.S., 2002, *Contaminant transport in fractured media: analytical solution and sensitivity study considering pulse, Dirac delta and sinusoid input sources*, Hydrological Processes 16[16], 3265-3278.

- Sudicky, E.A. and Frind, E.O., 1982, *Contaminant Transport in Fractured Porous-Media - Analytical Solutions for A System of Parallel Fractures*, Water Resources Research 18[6], 1634-1642.
- Sudicky, E.A. and Frind, E.O., 1984, *Contaminant Transport in Fractured Porous-Media - Analytical Solution for A 2-Member Decay Chain in A Single Fracture*, Water Resources Research 20[7], 1021-1029.
- Sun, Y.W. and Buscheck, T.A., 2003, *Analytical solutions for reactive transport of N-member radionuclide chains in a single fracture*, Journal of Contaminant Hydrology 62[3], 695-712.
- Tang, D.H., Frind, E.O., and Sudicky, E.A., 1981, *Contaminant Transport in Fractured Porous-Media - Analytical Solution for A Single Fracture*, Water Resources Research 17[3], 555-564.
- Troldborg, M., Lemming, G., Binning, P.J., Tuxen, N., and Bjerg, P.L., 2008, *Risk assessment and prioritisation of contaminated sites on the catchment scale*, Journal of Contaminant Hydrology 101[1-4], 14-28.
- US EPA, 1996, *Soil Screening Guidance: User's Guide*, Report Nr. 9355.4-23,
- US EPA, 2009, *EPA On-line Tools for Site Assessment Calculation*. <http://www.epa.gov/athens/learn2model/part-two/onsite/estdiffusion-ext.htm>
- van der Kamp, G. 1992. *Evaluating the effects of fractures on solute transport through fractured clayey aquitards*. Conference of the International Association of Hydrogeologists - Canadian National Chapter. Conference Proceeding
- van Genuchten, M.T. and Alves, W.J., 1982, *Analytical Solutions of the One Dimensional Convective-Dispersive Solute Transport Equation*, 1662. United States Department of Agriculture.Agricultural research Service.
- Videncenter for Jordforurening, 2008, *SprækkeJAGG - Regneark til risikovurdering af sprækker i moræneler*, GEO.

## **A risk assessment tool for contaminated sites in low-permeability fractured media**

In Denmark, many contaminated sites are located in areas with low permeability or fractured geologies such as glacial moraine clays. Fractures increase the risk of fast transport of contaminants to underlying groundwater systems. It is therefore important to consider fracture transport when evaluating the risk of contaminated sites to drinking water resources. This report describes the development of a fracture transport module for inclusion in the Danish EPA JAGG risk assessment tool.

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